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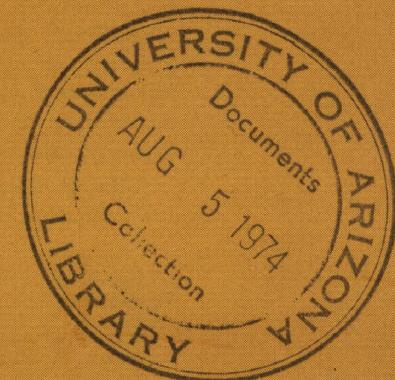
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NBS MONOGRAPH 25 — SECTION 11

Standard X-ray Diffraction Powder Patterns

U.S.
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National
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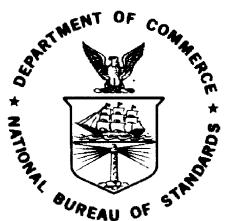
Standard X-ray Diffraction Powder Patterns

Section 11—Data for 70 Substances

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

Assisted by Johan H. de Groot and Simon J. Carmel

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**U.S. DEPARTMENT OF COMMERCE, Frederick B. Dent, Secretary
NATIONAL BUREAU OF STANDARDS, Richard W. Roberts, Director**

Issued February 1974

Library of Congress Catalog Number: 53—61386

National Bureau of Standards Monograph 25

Section 11—Data for 70 Substances

Nat. Bur. Stand. (U.S.), Monogr. 25—Sec. 11, 134 pages (Feb. 1974)

CODEN: NBSMA6

**U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON D.C.**

**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. 11). Price \$1.55**

CONTENTS

| | Page | | Page |
|---|-------------|---|-------------|
| Introduction..... | 1 | | |
| Experimental patterns: | | Calculated patterns: | |
| Aluminum bismuth oxide, $\text{Al}_4\text{Bi}_2\text{O}_9$ | 5 | Calcium bromide, CaBr_2 | 70 |
| Aluminum nitrate hydrate, $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ | 6 | Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ | 73 |
| Aluminum tungsten oxide, $\text{Al}_2(\text{WO}_4)_3$ | 7 | Chromium chloride, CrCl_2 | 77 |
| Ammonium copper fluoride, NH_4CuF_3 | 8 | Copper aluminum, Cu_9Al_4 | 79 |
| Ammonium formate, NH_4HCO_2 | 9 | Copper cadmium, Cu_5Cd_8 | 81 |
| Ammonium lead chloride, $(\text{NH}_4)_2\text{PbCl}_6$ | 10 | Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ | 83 |
| Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$ | 11 | Cysteine, L, $\text{HSCH}_2 \cdot \text{CH}(\text{NH}_2) \cdot \text{COOH}$ | 86 |
| Barium hydroxide phosphate, $\text{Ba}_5(\text{OH})(\text{PO}_4)_3$ | 12 | Iron fluoride hydrate, $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ | 90 |
| Barium lead chloride, BaPbCl_4 | 13 | Lithium hydroxide hydrate, $\text{LiOH} \cdot \text{H}_2\text{O}$ | 92 |
| Barium nitrate (nitrobarite), $\text{Ba}(\text{NO}_3)_2$ (revised)..... | 14 | Magnesium chloride (chloromagnesite), MgCl_2 | 94 |
| Cadmium bromide chloride, CdBrCl | 15 | Manganese oxide (partridgeite), alpha Mn_2O_3 (revised)..... | 95 |
| Calcium aluminum hydroxide, $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$.. | 16 | Manganese oxide hydroxide, groutite, alpha MnOOH | 97 |
| Calcium chloride (hydrophilite), CaCl_2 | 18 | Octahydro-1,3,5,7-tetranitro-1,3,5,7- tetrazocine (alpha HMX) $\text{C}_4\text{H}_8\text{N}_8\text{O}_8$ | 100 |
| Cesium cobalt chloride, Cs_2CoCl_4 | 19 | Octahydro-1,3,5,7-tetranitro-1,3,5,7- tetrazocine (beta HMX) $\text{C}_4\text{H}_8\text{N}_8\text{O}_8$ | 102 |
| Cesium copper chloride, Cs_2CuCl_4 | 20 | Potassium zinc bromide hydrate, $\text{KZnBr}_3 \cdot 2\text{H}_2\text{O}$ | 104 |
| Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$ | 22 | Potassium zinc iodide hydrate, $\text{KZnI}_3 \cdot 2\text{H}_2\text{O}$ | 107 |
| Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ | 23 | Sodium D-tartrate hydrate, $(\text{CHOH}-\text{CO}_2\text{Na})_2 \cdot 2\text{H}_2\text{O}$ | 110 |
| Cobalt fluoride hydrate, $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$ | 24 | Yttrium titanium oxide, Y_2TiO_5 | 113 |
| Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$ | 25 | | |
| Europium phosphate, EuPO_4 | 26 | | |
| Glucose, D, alpha, (dextrose), $\text{C}_6\text{H}_{12}\text{O}_6$ | 28 | | |
| Indium sulfide, In_2S_3 | 30 | | |
| Iron chloride hydrate, $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$ | 32 | | |
| Lead bromide chloride, PbBrCl | 33 | | |
| Magnesium bromide hydrate, $\text{MgBr}_2 \cdot 6\text{H}_2\text{O}$ | 35 | | |
| Magnesium chloride hydrate (bischofite), $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ | 37 | | |
| Manganese chloride hydrate, $\text{MnCl}_2 \cdot 2\text{H}_2\text{O}$ | 38 | | |
| Mercury ammine chloride, $\text{Hg}(\text{NH}_3)_2\text{Cl}_2$ | 39 | | |
| Neodymium phosphate, NdPO_4 | 40 | | |
| Nickel chloride hydrate, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ | 42 | Cumulative indices | |
| Nickel fluoride hydrate, $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$ | 43 | (Circular 539, Volumes 1-10 and Monograph 25, Sections 1-11) | |
| Potassium bromide iodide, $\text{KBr} \cdot 33\text{I} \cdot 67$ | 44 | | |
| Potassium bromide iodide, $\text{KBr} \cdot 67\text{I} \cdot 33$ | 45 | 1. Inorganic..... | 116 |
| Potassium cobalt fluoride, K_2CoF_4 | 46 | 2. Organic..... | 127 |
| Potassium tungsten oxide, K_2WO_4 | 47 | 3. Mineral..... | 128 |
| Sodium bromide chloride, $\text{NaBr} \cdot 33\text{Cl} \cdot 67$ | 49 | | |
| Sodium bromide chloride, $\text{NaBr} \cdot 67\text{Cl} \cdot 33$ | 50 | | |
| Sodium carbonate sulfate, $\text{Na}_4\text{CO}_3\text{SO}_4$ | 51 | | |
| Sodium carbonate sulfate (burkeite), $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ | 52 | | |
| Sodium carbonate sulfate, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ | 53 | | |
| Sodium carbonate sulfate, $\text{Na}_6(\text{CO}_3)_2\text{SO}_4$ | 54 | | |
| Sodium chromium oxide sulfate, $\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$ | 55 | | |
| Sodium magnesium carbonate (eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ | 56 | | |
| Sodium sulfate, Na_2SO_4 | 57 | | |
| Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$ | 58 | | |
| Strontium chloride hydroxide phosphate, $\text{Sr}_5\text{Cl} \cdot 65\text{OH} \cdot 35(\text{PO}_4)_3$ | 60 | | |
| Strontium oxide hydrate, $\text{SrO}_2 \cdot 8\text{H}_2\text{O}$ | 61 | | |
| Strontium phosphate, alpha $\text{Sr}_2\text{P}_2\text{O}_7$ | 62 | | |
| Strontium phosphate, alpha $\text{Sr}_3(\text{PO}_4)_2$ | 64 | | |
| Sucrose, $\text{C}_{12}\text{H}_{22}\text{O}_11$ | 66 | | |
| Zinc ammine bromide, $\text{Zn}(\text{NH}_3)_2\text{Br}_2$ | 68 | | |
| Zinc fluoride hydrate, $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ | 69 | | |

Errata

Circular 539

Volume 2, page 30. In column 2, the density of PbO (red) should be 9.334 g/cm³.

Volume 4, page 60. In the table column 4, the d-spacing 3.36 should be 2.36.

Volume 6, page 60. In the table column 2, the d-spacing 2.75 should be 1.75.

Volume 7, page 29. In the table, the NBS d-spacing 1.426 should be 1.406.

Monograph 25

Section 4, page 31. In the reference 4, the formula should be KC₆H₄COOH-COO.

Section 7, page 2 } In each section, the formula for L_p should be:

Section 8, page 3 }

Section 9, page 3 }

Section 10, page 3 }

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

Section 8, page 3. The formula for B should be:

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

Section 9, page 115. The index entry for ammonium chloroosmate, (NH₄)₂OsCl₆, should be Sec. 1m, pg. 6.

Section 10, page 11. In the sample description, line 2, BrF₂ should be BaF₂.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

The following copies may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, Virginia, 22151. Where these publications are identified with a number, it must be used in ordering. They are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

| NBS Publication | Number | NBS Publication | Number |
|-----------------------------|------------|------------------------------|--------------|
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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 11. --- Data for 70 Substances

by

Howard E. Swanson, Howard F. McMurdie,¹ Marlene C. Morris²
Eloise H. Evans,² and Boris Paretzkin²
Assisted by Johan H. de Groot² and Simon J. Carmel

Standard x-ray diffraction patterns are presented for 70 substances. Fifty-two of these patterns represent experimental data and 18 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

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

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the Joint Committee on Powder Diffraction Standards,³ the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the Joint Committee, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 70 compounds (52 experimental and 18 calculated patterns), and is the twenty-first of the series of "Standard X-ray Diffraction Powder Patterns."⁴

EXPERIMENTAL POWDER PATTERNS

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

Optical data, 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].

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

³Joint 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.

⁴See previous page for other published volumes.

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

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 $\lambda = 1.54056 \text{ \AA}$

| hkl | W $a = 3.16516 \text{ \AA}$ $\pm .00004$ | Ag $a = 4.08641 \text{ \AA}$ $\pm .00002$ |
|-------|--|---|
| 110 | 40.262° | |
| 111 | | 38.112° |
| 200 | 58.251 | 44.295 |
| 211 | 73.184 | |
| 220 | 86.996 | 64.437 |
| 310 | 100.632 | |
| 311 | | 77.390 |
| 222 | 114.923 | 81.533 |
| 321 | 131.171 | |
| 400 | 153.535 | 97.875 |
| 331 | | 110.499 |
| 420 | | 114.914 |
| 422 | | 134.871 |
| 511 | | 156.737 |

All of our spacing measurements were recorded at $25 \pm 1 \text{ }^{\circ}\text{C}$ on a diffractometer equipped with a curved lithium fluoride crystal monochromator located between the sample and the Geiger counter. Copper radiation was used and the wavelength K α_1 was taken to be 1.54056 \AA [Bearden, 1964].

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 using a cell with the three shortest edges [Crystal Data, Vol. II, 1973].

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 $\sum(\theta_{\text{obs}} - \theta_{\text{calc}})^2$. 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. Beginning with this issue, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertain-

ty 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 NBS determined lattice constants, the Avogadro number (6.02252×10^{23}), 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 $10 \mu\text{m}$, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (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.

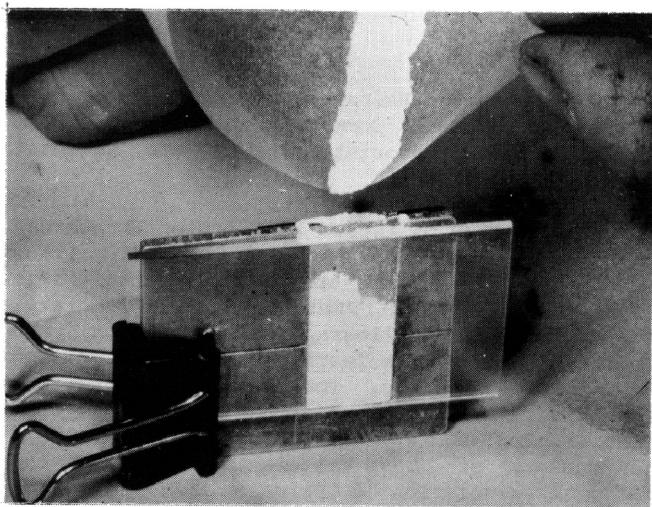


Figure 1

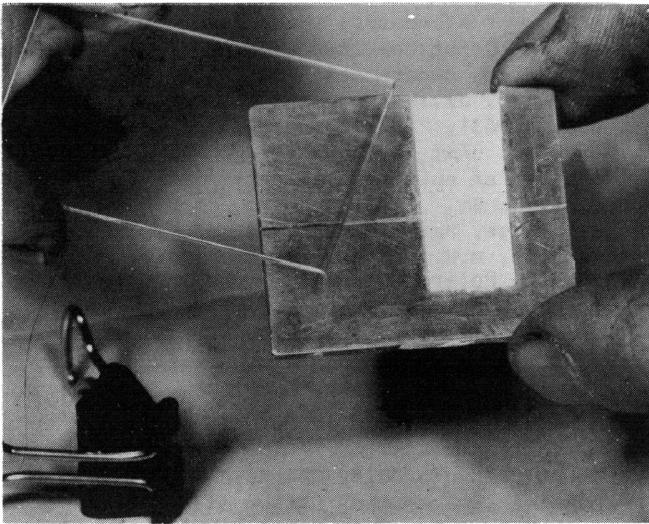


Figure 2

Reference intensity, 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 and 2), and the pattern was taken. The reference intensity was then calculated as the direct ratio of the strongest line of the sample to the strongest line of corundum (hexagonal 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 Smith [1967] and modified at NBS.

Lattice parameters. Before the computations of the patterns, changes were made as necessary in the lattice constants in order to make them consistent with the revised value of the copper wavelength [Bearden, 1964]; specifically, a published lattice constant in Å was multiplied by 1.00004. Both the altered parameter and the original published value are given. Monoclinic and triclinic lattice constants were transformed if necessary, to follow the convention of using a cell with the 3 shortest edges [Crystal Data, Vol. II, 1973].

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

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

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, in place of using given anisotropic parameters, approximately equivalent isotropic values were substituted as defined by:

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

Integrated intensities. Intensity calculations were based on the copper $K\alpha_1$ wavelength, 1.54056 Å, determined by Bearden [1964]. The integrated intensities were computed from formula (1):

$$(1) \quad I = F^2 (L_p) (FAC)$$

where F is the standard structure factor

FAC is the powder multiplicity

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

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

Scale factor. For each compound, this factor multiplied by the reported integrated intensities will reproduce the unscaled intensities which were derived using formula (1).

Peak intensities. The integrated intensities can be transformed to a Cauchy profile with an appropriate variable half-width designated to simulate a diffractometer tracing [Smith, 1967]. The value of the half-width was chosen as 0.075° at 40° (2θ , CuK α_1). Then the intensities were summed for the overlapping peak profiles, and the resulting new peak intensities were scaled to the strongest peak height which was assigned a value of 100. Reflections were not reported which had scaled peak heights of 0.7 or less. Adjacent peaks with nearly equal 2θ values usually cannot be experimentally resolved; therefore one composite peak was calculated in such instances. The 2θ angle of this peak was assigned the hkl of the reflection having the greatest integrated intensity; a plus sign (+) was used to indicate additional hkl 's.

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Aluminum bismuth oxide, $\text{Al}_4\text{Bi}_2\text{O}_9$

Sample

The sample was prepared by heating a 2:1 mixture of $\alpha\text{Al}_2\text{O}_3$ and Bi_2O_3 at 1000 °C. This was followed by grinding and reheating.

Color

Pale yellow

Structure

Orthorhombic, Pbam (55), $Z=2$, isostructural with $\text{Bi}_2\text{Ga}_4\text{O}_9$. The structure was determined by Eckerlin and Liebertz [1965].

NBS lattice constants:.

$$a = 7.719(1)\text{\AA}$$

$$b = 8.109(1)$$

$$c = 5.6919(8)$$

Density
(calculated) 6.244 g/cm^3

Reference intensity
 $I/I_{\text{corundum}} = 3.1$

Additional patterns

1. PDF card 23-1006 [Surnina and Litvin, 1970].

References

Eckerlin, P. and Liebertz, J. (1965). Naturwissenschaften 52, 540.

Surnina, V.S. and Litvin, B.N. (1970). Soviet Phys. Cryst. English Transl. 15, 527.

Internal standard Ag, $a = 4.08641 \text{ \AA}$

$\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C

| $d (\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
|------------------|-----|-------|-------------------|
| 5.68 | 75 | 001 | 15.58 |
| 4.055 | 12 | 020 | 21.90 |
| 3.989 | 5 | 111 | 22.27 |
| 3.862 | 10 | 200 | 23.01 |
| 3.591 | 35 | 120 | 24.77 |
| 3.485 | 25 | 210 | 25.54 |
| 3.301 | 19 | 021 | 26.99 |
| 3.192 | 20 | 201 | 27.93 |
| 3.034 | 100 | 121 | 29.41 |
| 2.971 | 85 | 211 | 30.05 |

| $d (\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
|------------------|-----|----------|-------------------|
| 2.846 | 30 | 002 | 31.41 |
| 2.795 | 12 | 220 | 32.00 |
| 2.551 | 15 | 130 | 35.15 |
| 2.537 | 14 | 112 | 35.35 |
| 2.510 | 3 | 221 | 35.75 |
| 2.453 | 9 | 310 | 36.60 |
| 2.328 | 16 | 022, 131 | 38.65 |
| 2.290 | 14 | 202 | 39.31 |
| 2.252 | 11 | 311 | 40.01 |
| 2.230 | 12 | 122 | 40.42 |
| 2.204 | 35 | 212 | 40.91 |
| 2.028 | 1 | 321, 040 | 44.64 |
| 1.994 | 1 | 222 | 45.44 |
| 1.961 | 12 | 140 | 46.26 |
| 1.930 | 3 | 400 | 47.05 |
| 1.908 | 2 | 041 | 47.61 |
| 1.898 | 10 | 132, 003 | 47.88 |
| 1.878 | 7 | 410 | 48.44 |
| 1.864 | 15 | 330 | 48.83 |
| 1.857 | 16 | 312 | 49.02 |
| 1.854 | 25 | 141 | 49.10 |
| 1.827 | 1 | 401 | 49.87 |
| 1.795 | 3 | 240 | 50.82 |
| 1.783 | 16 | 411 | 51.18 |
| 1.771 | 17 | 331 | 51.55 |
| 1.743 | 3 | 420 | 52.46 |
| 1.726 | 1 | 322 | 53.00 |
| 1.719 | 2 | 023 | 53.25 |
| 1.703 | 2 | 203 | 53.77 |
| 1.677 | 14 | 123 | 54.69 |
| 1.666 | 13 | 213, 421 | 55.07 |
| 1.652 | 5 | 042 | 55.60 |
| 1.615 | 7 | 142 | 56.98 |
| 1.597 | 5 | 402 | 57.66 |
| 1.567 | 9 | 412 | 58.87 |
| 1.559 | 25 | 332 | 59.21 |
| 1.528 | 1 | 151 | 60.54 |
| 1.5222 | 2 | 133 | 60.80 |
| 1.5004 | 2 | 313 | 61.78 |
| 1.4954 | 2 | 250 | 61.98 |
| 1.4655 | 1 | 511 | 63.42 |
| 1.4465 | 6 | 251 | 64.35 |
| 1.4233 | 5 | 004 | 65.53 |
| 1.3989 | 6 | 521 | 66.82 |
| 1.3865 | 3 | 152 | 67.50 |
| 1.3722 | 2 | 350 | 68.30 |
| 1.3638 | 5 | 143 | 68.78 |

Aluminum nitrate hydrate, $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation of an aqueous solution of $\text{Al}(\text{NO}_3)_3$. The crystals were filtered out and washed with ethyl alcohol.

Color

Colorless

Optical data

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

Structure

Monoclinic, $P2_1/c$ (14), $Z=4$, isostructural with $\text{Cr}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ [Kannan and Viswamitra, 1965].

NBS lattice constants:

$a = 13.847(8)\text{\AA}$
 $b = 9.617(2)$
 $c = 10.908(5)$
 $\beta = 95.68(2)^\circ$

Density

(calculated) 1.724 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 0.5$

Additional patterns

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

References

- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Kannan, K. K. and Viswamitra, M. A. (1965). Acta Cryst. 19, 151.

| Internal standard W, $a = 3.16516 \text{ \AA}$ | | | |
|---|-----|---------|-------------------|
| $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
| $d (\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
| 7.87 | 1 | 110 | 11.24 |
| 7.20 | 12 | 011 | 12.29 |
| 6.55 | 70 | 111 | 13.51 |
| 6.21 | 60 | 111 | 14.26 |
| 5.60 | 14 | 210 | 15.81 |
| 5.22 | 6 | 102 | 16.97 |
| 4.89 | 18 | 102 | 18.13 |
| 4.82 | 25 | 211,020 | 18.41 |
| 4.729 | 4 | 012 | 18.75 |
| 4.595 | 4 | 112,300 | 19.30 |

| $d (\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
|------------------|-----|-----------|-------------------|
| 4.539 | 15 | 120 | 19.54 |
| 4.487 | 45 | 202 | 19.77 |
| 4.362 | 3 | 112 | 20.34 |
| 4.231 | 2 | 121 | 20.98 |
| 4.143 | 10 | 310,121 | 21.43 |
| 4.074 | 60 | 202 | 21.80 |
| 3.994 | 45 | 311 | 22.24 |
| 3.943 | 50 | 220 | 22.53 |
| 3.762 | 30 | 311 | 23.63 |
| 3.639 | 12 | 221 | 24.44 |
| 3.599 | 65 | 022 | 24.72 |
| 3.541 | 6 | 122 | 25.13 |
| 3.449 | 9 | 312,400 | 25.81 |
| 3.426 | 12 | 122 | 25.99 |
| 3.387 | 6 | 013 | 26.29 |
| 3.278 | 16 | 222 | 27.18 |
| 3.244 | 35 | 410,321 | 27.47 |
| 3.219 | 19 | 113 | 27.69 |
| 3.123 | 20 | 130 | 28.56 |
| 3.112 | 20 | 321 | 28.66 |
| 3.074 | 12 | 031 | 29.02 |
| 3.049 | 20 | 402 | 29.27 |
| 3.017 | 100 | 131 | 29.58 |
| 2.982 | 45 | 131 | 29.93 |
| 2.907 | 35 | 230,412 | 30.73 |
| 2.878 | 7 | 123 | 31.05 |
| 2.854 | 5 | 313 | 31.32 |
| 2.835 | 4 | 231 | 31.53 |
| 2.788 | 3 | 402,123 | 32.08 |
| 2.779 | 7 | 231 | 32.18 |
| 2.761 | 18 | 032 | 32.40 |
| 2.680 | 6 | 132 | 33.41 |
| 2.615 | 20 | 204,104,+ | 34.26 |
| 2.609 | 30 | 014,232,+ | 34.34 |
| 2.590 | 50 | 331 | 34.60 |
| 2.538 | 16 | 323 | 35.33 |
| 2.522 | 35 | 331,114,+ | 35.57 |
| 2.446 | 3 | 304,204 | 36.71 |
| 2.422 | 2 | 332 | 37.09 |
| 2.399 | 6 | 033 | 37.45 |
| 2.393 | 4 | 520,133 | 37.56 |
| 2.369 | 40 | 314,140,+ | 37.95 |
| 2.363 | 25 | 124,024,+ | 38.05 |
| 2.348 | 30 | 041,430 | 38.31 |
| 2.326 | 4 | 431 | 38.68 |
| 2.307 | 12 | 423,141 | 39.01 |
| 2.301 | 14 | 224,600,+ | 39.16 |
| 2.271 | 16 | 240 | 39.65 |
| 2.263 | 8 | 431,522 | 39.80 |
| 2.242 | 10 | 404,513,+ | 40.19 |
| 2.210 | 2 | 432,241 | 40.79 |
| 2.184 | 16 | 142,414,+ | 41.30 |

Aluminum tungsten oxide, $\text{Al}_2(\text{WO}_4)_3$

Sample

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

Color

Colorless

Structure

Orthorhombic, Pnca (60), $Z=2$, isostructural with other tungstates and molybdates of the smaller trivalent rare-earth elements such as $\text{Gd}_2(\text{WO}_4)_3$ [Craig and Stephenson, 1968].

NBS lattice constants:

$$\begin{aligned} a &= 9.139(2) \text{\AA} \\ b &= 12.596(2) \\ c &= 9.060(2) \end{aligned}$$

Density
(calculated) 2.539 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 2.3$$

Additional patterns

- PDF card 18-72 [Waring, 1965] (incorrectly called $2\text{Al}_2\text{O}_3 \cdot 5\text{WO}_3$)

References

Craig, D. C. and Stephenson, N. C. (1968). Acta Cryst. B24, 1250.
Waring, J. (1965). J. Am. Ceram. Soc. 48, 493.

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

| $\overset{\circ}{\text{Internal standard W, a = 3.16516 Å}}$ | | | |
|---|-----|-------|---------------|
| $\text{CuK}\alpha_1 \lambda = 1.54056 \text{\AA}; \text{temp. } 25^\circ\text{C}$ | | | |
| d (Å) | I | hkl | 2θ (°) |
| 6.30 | 11 | 020 | 14.04 |
| 5.73 | 13 | 111 | 15.46 |
| 4.53 | 11 | 002 | 19.59 |
| 4.50 | 6 | 121 | 19.73 |
| 4.296 | 35 | 210 | 20.66 |
| 4.059 | 40 | 102 | 21.88 |
| 3.877 | 50 | 211 | 22.92 |
| 3.867 | 45 | 112 | 22.98 |
| 3.810 | 100 | 031 | 23.33 |
| 3.697 | 16 | 220 | 24.05 |

Ammonium copper fluoride, NH_4CuF_3

Sample

The sample was prepared by the reaction of Cu and Br in methanol; the product was added to a saturated methanol solution of NH_4HF_2 . The precipitate was filtered, and washed with methanol and ether. The sample was somewhat hygroscopic.

Color

Greenish white

Structure

Tetragonal, P4mm (99), $Z=2$, similar to KCuF_3 , distorted perovskite. Crockett and Haendler [1960] gave a larger cell related to ours as $a \approx a\sqrt{2}$ and $c \approx 2c$. We found no lines which required the larger cell.

NBS lattice constants:

$$a = 6.0828(4)\text{\AA}$$

$$c = 3.8915(4)$$

Density
(calculated) 3.196 g/cm^3

Reference intensity

$$I/I_{\text{conundum}} = 2.4$$

Additional patterns

1. PDF card 22-41 [Clavan, 1969, Pennwalt Corp. King of Prussia, Penna.]

References

Crockett, D.S. and Haendler, H.M. (1960). J. Am. Chem. Soc. 82, 4158.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}$; temp. 25° C | | | |
|--|-----|----------|---------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 4.300 | 100 | 110 | 20.64 |
| 3.889 | 35 | 001 | 22.85 |
| 3.041 | 35 | 200 | 29.35 |
| 2.885 | 55 | 111 | 30.97 |
| 2.719 | 4 | 210 | 32.92 |
| 2.395 | 3 | 201 | 37.52 |
| 2.230 | 4 | 211 | 40.42 |
| 2.150 | 50 | 220 | 41.98 |
| 1.946 | 19 | 002 | 46.64 |
| 1.924 | 18 | 310 | 47.20 |
| 1.882 | 15 | 221 | 48.31 |
| 1.773 | 15 | 112 | 51.50 |
| 1.725 | 14 | 311 | 53.05 |
| 1.640 | 8 | 202 | 56.04 |
| 1.5478 | 2 | 321 | 59.69 |
| 1.5208 | 9 | 400 | 60.86 |
| 1.4753 | 3 | 410 | 62.95 |
| 1.4429 | 17 | 222 | 64.53 |
| 1.4336 | 5 | 330 | 65.00 |
| 1.4166 | 5 | 401 | 65.88 |
| 1.3681 | 9 | 312 | 68.53 |
| 1.3601 | 5 | 420 | 68.99 |
| 1.3453 | 4 | 331 | 69.86 |
| 1.2970 | 2 | 003 | 72.87 |
| 1.2419 | 4 | 113 | 76.67 |
| 1.1983 | 6 | 402 | 80.00 |
| 1.1930 | 5 | 203, 510 | 80.43 |
| 1.1755 | 2 | 412 | 81.88 |
| 1.1542 | 5 | 332 | 83.73 |
| 1.1407 | 5 | 511 | 84.95 |
| 1.1146 | 4 | 422 | 87.43 |
| 1.1109 | 3 | 223 | 87.80 |
| 1.0756 | 4 | 313, 440 | 91.47 |
| 1.0169 | 4 | 512 | 98.48 |

Ammonium formate, HCOONH₄

Sample

The sample was obtained from the K and K Laboratories, Inc., Jamaica, N.Y. The material was somewhat hygroscopic.

Color

Colorless

Structure

Monoclinic, P_C (7), Z=2. The structure was determined by Nahringbauer [1968].

NBS lattice constants

a = 3.8202(5) Å
b = 4.6816(6)
c = 9.118(1)
β = 91.12(1) °

Density
(calculated) 1.284 g/cm³

Reference intensity

I/I_{corundum} = 1.5

Additional patterns

1. PDF card 14-756 [Hanawalt et al., 1938]

References

Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938).
Ind. Eng. Chem. Anal. Ed. 10, 457.
Nahringbauer, I. (1968). Acta Cryst. B24, 565.

| Internal standard W, a = 3.16516 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C | | | |
|--|-----|----------|--------|
| d (Å) | I | hkl | 2° (°) |
| 4.555 | 55 | 002 | 19.47 |
| 4.164 | 65 | 011 | 21.32 |
| 3.819 | 10 | 100 | 23.27 |
| 3.266 | 14 | 012 | 27.28 |
| 2.954 | 100 | 110, 102 | 30.23 |
| 2.898 | 5 | 102 | 30.83 |
| 2.826 | 30 | 111 | 31.63 |
| 2.802 | 6 | 111 | 31.91 |
| 2.550 | 9 | 013 | 35.17 |
| 2.500 | 10 | 112 | 35.89 |
| 2.466 | 9 | 112 | 36.41 |
| 2.340 | 8 | 020 | 38.43 |
| 2.279 | 13 | 004 | 39.51 |
| 2.267 | 11 | 021 | 39.73 |
| 2.137 | 2 | 113 | 42.26 |
| 2.105 | 1 | 113 | 42.92 |
| 2.083 | 4 | 022 | 43.41 |
| 2.049 | 7 | 014 | 44.16 |
| 1.996 | 1 | 120 | 45.39 |
| 1.974 | 4 | 104 | 45.93 |
| 1.955 | 1 | 121 | 46.42 |
| 1.945 | 2 | 121 | 46.66 |
| 1.941 | 1 | 104 | 46.76 |
| 1.9095 | 1 | 200 | 47.58 |
| 1.8546 | 4 | 023 | 49.08 |
| 1.8350 | 1 | 122 | 49.64 |
| 1.8192 | 2 | 114 | 50.10 |
| 1.7932 | <1 | 114 | 50.88 |
| 1.7733 | 2 | 202 | 51.49 |
| 1.7685 | 2 | 210 | 51.64 |
| 1.7490 | 1 | 202 | 52.26 |
| 1.7419 | 1 | 211 | 52.49 |
| 1.7296 | 1 | 211 | 52.89 |
| 1.6990 | 2 | 015 | 53.92 |
| 1.6758 | 2 | 123 | 54.73 |
| 1.6598 | 2 | 123, 212 | 55.30 |
| 1.6335 | <1 | 105, 024 | 56.27 |
| 1.5635 | 2 | 115 | 59.03 |
| 1.5406 | 2 | 213 | 60.00 |
| 1.5380 | 2 | 031 | 60.11 |
| 1.5193 | 1 | 006 | 60.93 |
| 1.5085 | 1 | 124 | 61.41 |
| 1.4938 | <1 | 124 | 62.08 |
| 1.4801 | <1 | 220 | 62.72 |
| 1.4767 | 1 | 032 | 62.88 |
| 1.4646 | 1 | 221 | 63.46 |
| 1.4574 | 1 | 221 | 63.81 |
| 1.4451 | 1 | 016, 130 | 64.42 |
| 1.4283 | 2 | 131 | 65.27 |
| 1.4246 | 2 | 131 | 65.46 |

Ammonium lead chloride, $(\text{NH}_4)_2\text{PbCl}_6$

Sample

Chlorine was bubbled through a saturated solution of PbCl_2 in concentrated HCl. Then a saturated solution of NH_4Cl in concentrated HCl was added. The precipitate formed was filtered without washing.

Color

Brilliant green yellow

Structure

Cubic, $\text{Fm}3\text{m}$ (225), $Z=4$, isostructural with K_2PtCl_6 . The structure was determined by Wyckoff and Dennis [1926].

NBS lattice constant:
 $a = 10.1609(3)\text{\AA}$

Density

(calculated) 2.887 g/cm^3

Reference intensity

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

Additional patterns

1. PDF card 2-0139 [Wyckoff and Dennis, 1926].

Reference

Wyckoff, R. W. G. and Dennis, L. M. (1926). Am. J. Sci. 12, 503.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
|---|-----|-------|-------------------------|
| $d (\text{\AA})$ | I | hkl | $2\psi (\text{)}^\circ$ |
| 5.866 | 100 | 111 | 15.09 |
| 5.081 | 45 | 200 | 17.44 |
| 3.593 | 20 | 220 | 24.76 |
| 3.061 | 45 | 311 | 29.15 |
| 2.933 | 1 | 222 | 30.45 |
| 2.540 | 25 | 400 | 35.31 |
| 2.332 | 18 | 331 | 38.57 |
| 2.272 | 25 | 420 | 39.63 |
| 2.074 | 9 | 422 | 43.61 |
| 1.955 | 14 | 511 | 46.41 |
| 1.796 | 15 | 440 | 50.78 |
| 1.718 | 12 | 531 | 53.29 |
| 1.693 | 10 | 600 | 54.11 |
| 1.607 | 2 | 620 | 57.28 |
| 1.5495 | 4 | 533 | 59.62 |
| 1.4667 | 3 | 444 | 63.36 |
| 1.4229 | 4 | 711 | 65.55 |
| 1.4090 | 2 | 640 | 66.28 |
| 1.3577 | 2 | 642 | 69.13 |
| 1.3227 | 4 | 731 | 71.23 |
| 1.2701 | <1 | 800 | 74.67 |
| 1.2415 | 1 | 733 | 76.70 |
| 1.2324 | 3 | 820 | 77.37 |
| 1.1976 | 1 | 822 | 80.06 |
| 1.1733 | 2 | 751 | 82.07 |
| 1.1359 | 2 | 840 | 85.39 |
| 1.1152 | 2 | 911 | 87.37 |
| 1.1087 | 2 | 842 | 88.02 |
| 1.0829 | <1 | 664 | 90.68 |
| 1.0652 | 1 | 931 | 92.63 |
| 1.0369 | 1 | 844 | 95.95 |
| 1.0211 | 2 | 933 | 97.94 |
| 1.0161 | 1 | 10000 | 98.59 |
| 0.9964 | 1 | 10200 | 101.25 |
| 0.9823 | 1 | 951 | 103.28 |

Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution containing 2 grams NH_4Cl and 3.6 grams $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$. The first crystals formed were used. The method follows the phase study of the $\text{NH}_4\text{Cl}-\text{MnCl}_2-\text{H}_2\text{O}$ system by Clendinnen and Rivett [1921].

Color

Pinkish white

Structure

Tetragonal, $P4_2/mnm$ (136), $Z=2$, isostructural with $(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ [Greenberg and Walden, 1940]. The structure of $(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ was determined by Hendricks and Dickerson [1927] and refined by Chrobak, [1934]. Greenberg and Walden [1940] found $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$ to have a solid solution relation with $(\text{NH}_4)_6\text{MnCl}_8 \cdot 2\text{H}_2\text{O}$.

NBS lattice constants:

$$a = 7.589(1) \text{\AA}$$

$$c = 8.143(2)$$

Density

(calculated) 1.904 g/cm^3

Reference intensity

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

| $d (\text{\AA})$ | I | Internal standard Ag, $a = 4.08641 \text{ \AA}$ | |
|------------------|-----|---|---------------------------|
| | | hkl | $2\theta (\text{)}^\circ$ |
| 5.552 | 35 | 101 | 15.95 |
| 5.365 | 15 | 110 | 16.51 |
| 4.073 | 35 | 002 | 21.80 |
| 3.797 | 6 | 200 | 23.41 |
| 3.244 | 8 | 112 | 27.47 |
| 3.131 | 8 | 211 | 28.48 |
| 2.776 | 100 | 202 | 32.22 |
| 2.684 | 90 | 220 | 33.36 |
| 2.557 | 8 | 103 | 35.06 |
| 2.401 | 4 | 310 | 37.43 |
| 2.240 | 25 | 222 | 40.22 |
| 2.120 | 5 | 213 | 42.61 |
| 2.067 | 1 | 312 | 43.76 |
| 2.038 | 19 | 321 | 44.41 |
| 1.898 | 16 | 400 | 47.89 |
| 1.798 | 3 | 313 | 50.72 |
| 1.7938 | 5 | 204 | 50.86 |
| 1.7194 | 8 | 402 | 53.23 |
| 1.6629 | 4 | 323 | 55.19 |
| 1.6213 | 17 | 224 | 56.73 |
| 1.5660 | 9 | 422 | 58.93 |
| 1.5231 | 2 | 413 | 60.76 |
| 1.4923 | 2 | 431 | 62.15 |
| 1.3877 | 8 | 521,404 | 67.43 |

References

- Chrobak, L. (1934). Z. Krist. **88**, 35.
 Clendinnen, F.W.J. and Rivett, A.C.D. (1921). J. Chem. Soc. **119**, 1329.
 Greenberg, A.L. and Walden, G. H. Jr. (1940). J. Chem. Phys. **8**, 645.
 Hendricks, S.B. and Dickerson, R.G. (1927). J. Am. Chem. Soc. **49**, 2149.

Additional patterns

1. PDF card 2-844 [Greenberg and Walden, 1940].

Barium hydroxide phosphate, $\text{Ba}_5(\text{OH})(\text{PO}_4)_3$

Sample

The sample was prepared by heating $\text{Ba}(\text{OH})_2$ and $(\text{NH}_4)_2\text{HPO}_4$ together in a molar ratio of 5 : 3. After heating at 300 °C, the material was pelletized and reheated at 600 °C for one hour, at 900 °C for one hour, and at 1100 °C for one half hour.

Color

Colorless

Structure

Hexagonal, $P6_3/m$ (176), $Z=2$, isostructural with calcium and lead hydroxyapatites [Klement and Dihn, 1938]. The structure of $\text{Ca}_5(\text{OH})(\text{PO}_4)_3$ was refined by Posner et al. [1958].

NBS lattice constants:

$$a = 10.185(1) \text{\AA}$$

$$c = 7.729(1)$$

Density

(calculated) 4.728 g/cm³

Reference intensity

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

Additional patterns

1. PDF card 1-811 [Hanawalt et al., 1938]
2. PDF card 3-578 [Klement and Dihn, 1938]

References

- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
 Klement, R. and Dihn, P. (1938). Z. anorg. u. allgem. Chem. 240, 40.
 Posner, A.S., Perloff, A., and Diorio, A.F. (1958). Acta Cryst. 11, 308.

| Internal standard W, $a = 3.16516 \text{\AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|--|-----|-------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 5.10 | 3 | 110 | 17.37 |
| 4.410 | 25 | 200 | 20.12 |
| 4.255 | 19 | 111 | 20.86 |
| 3.869 | 12 | 002 | 22.97 |
| 3.829 | 1 | 201 | 23.21 |
| 3.541 | 30 | 102 | 25.13 |
| 3.334 | 35 | 210 | 26.72 |
| 3.079 | 100 | 112 | 28.98 |
| 3.062 | 100 | 211 | 29.14 |
| 2.940 | 50 | 300 | 30.38 |
| 2.908 | 4 | 202 | 30.72 |
| 2.546 | 2 | 220 | 35.22 |
| 2.447 | 8 | 310 | 36.70 |
| 2.338 | 5 | 302 | 38.47 |
| 2.334 | 2 | 311 | 38.54 |
| 2.299 | 11 | 113 | 39.15 |
| 2.225 | 2 | 203 | 40.50 |
| 2.205 | 3 | 400 | 40.90 |
| 2.127 | 30 | 222 | 42.47 |
| 2.067 | 25 | 312 | 43.76 |
| 2.038 | 30 | 213 | 44.41 |
| 2.023 | 6 | 320 | 44.77 |
| 1.958 | 17 | 321 | 46.34 |
| 1.932 | 12 | 004 | 47.00 |
| 1.925 | 20 | 410 | 47.18 |
| 1.915 | 25 | 402 | 47.43 |
| 1.868 | 1 | 411 | 48.70 |
| 1.807 | 1 | 114 | 50.45 |
| 1.792 | <1 | 322 | 50.91 |
| 1.775 | 1 | 313 | 51.45 |
| 1.769 | 3 | 204 | 51.62 |
| 1.7230 | 3 | 412 | 53.11 |
| 1.6979 | <1 | 330 | 53.96 |
| 1.6721 | 10 | 214 | 54.86 |
| 1.6671 | 8 | 420 | 55.04 |
| 1.6582 | 3 | 331 | 55.36 |
| 1.6290 | 1 | 421 | 56.44 |
| 1.6143 | 8 | 304 | 57.00 |
| 1.6048 | 5 | 502 | 57.37 |
| 1.5913 | 8 | 323 | 57.90 |

Barium lead chloride, BaPbCl₄

Sample

The sample was prepared by melting an equimolar mixture of BaCl₂ and PbCl₂. It was then ground and heated for 18 hours, at 400 °C, in a sealed glass tube. This was repeated twice.

Color

Colorless

Structure

Orthorhombic, Pnam (62), Z = 2; BaCl₂ and PbCl₂ form a complete solid solution series [Calingaert et al., 1949]. The structure of BaCl₂ was determined by Döll and Klemm [1939] and refined by Brackett et al. [1963] and Sahl [1963].

NBS lattice constant:

$$a = 7.765(2) \text{ \AA}$$

$$b = 9.246(2)$$

$$c = 4.658(1)$$

Density (calculated) 4.829 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 2.8$$

References

- Brackett, E. B., Brackett, T. E., and Sass, R. L. (1963). J. Phys. Chem. 67, 2132.
- Calingaert, G., Lamb, F. W., and Meyer, F. (1949). J. Am. Chem. Soc. 71, 3712.
- Döll, W. and Klemm, W. (1939). Z. anorg. u. allgem. Chem. 241, 239.
- Sahl, K. (1963). Beitr. Mineral. Petrog. 9, 111.

| Internal standard W, a = 3.16516 Å $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|--|----------|------------|--------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2</i> (°) |
| 4.62 | 11 | 020 | 19.20 |
| 4.16 | 40 | 011 | 21.35 |
| 3.97 | 95 | 120 | 22.40 |
| 3.885 | 55 | 200 | 22.87 |
| 3.664 | 100 | 111 | 24.27 |
| 3.020 | 13 | 121 | 29.55 |
| 2.981 | 14 | 201 | 29.95 |
| 2.972 | 20 | 220 | 30.04 |
| 2.866 | 11 | 130 | 31.18 |
| 2.838 | 80 | 211 | 31.50 |
| 2.572 | 50 | 031 | 34.86 |
| 2.508 | 4 | 221 | 35.77 |
| 2.440 | 12 | 131 | 36.80 |
| 2.415 | 5 | 230 | 37.20 |
| 2.331 | 30 | 002 | 38.60 |
| 2.311 | 19 | 040 | 38.94 |
| 2.259 | 35 | 320 | 39.87 |
| 2.215 | 7 | 140 | 40.70 |
| 2.197 | 35 | 311 | 41.05 |
| 2.142 | 40 | 231 | 42.15 |
| 2.081 | 2 | 022 | 43.45 |
| 2.009 | 20 | 122 | 45.08 |
| 1.997 | 17 | 202 | 45.38 |
| 1.986 | 11 | 240 | 45.63 |
| 1.941 | 7 | 400 | 46.76 |
| 1.833 | 3 | 222 | 49.71 |
| 1.759 | 2 | 411 | 51.94 |
| 1.678 | 10 | 151 | 54.64 |
| 1.675 | 7 | 232 | 54.76 |
| 1.642 | 7 | 430 | 55.96 |
| 1.6216 | 15 | 322 | 56.72 |
| 1.6053 | 3 | 142 | 57.35 |
| 1.5720 | <1 | 251 | 58.68 |
| 1.5492 | 4 | 431 | 59.63 |
| 1.5110 | 6 | 242 | 61.30 |
| 1.5023 | 5 | 113 | 61.69 |
| 1.4910 | 5 | 402 | 62.21 |
| 1.4869 | 5 | 440 | 62.40 |
| 1.4556 | 7 | 511 | 63.90 |
| 1.4318 | 8 | 351 | 65.09 |

Barium nitrate (nitrobarite), $\text{Ba}(\text{NO}_3)_2$ (revised)

Sample

The sample was specially purified material from Mallinckrodt Chemical Works, New York.

Major impurities

0.001-0.01% each: Al, Na, and Sr.

Color

Colorless

Optical data

Isotropic, $N = 1.571$

Structure

Cubic, $P2_13$ (198), $Z = 4$, isostructural with $\text{Sr}(\text{NO}_3)_2$. The structure was determined by Birnstock [1967]. Previously the space group of $\text{Ba}(\text{NO}_3)_2$ was considered to be $\text{Pa}3$ (205).

NBS lattice constant:

$$a = 8.1184(2) \text{\AA}$$

Density

(calculated) 3.244 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 4.5$$

Additional patterns

1. PDF card 4-773 [Swanson and Tatge, 1953]

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25° C | | | |
|---|-----|-------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2^\circ (\text{ })$ |
| 4.689 | 100 | 111 | 18.91 |
| 4.062 | 35 | 200 | 21.86 |
| 3.633 | 14 | 210 | 24.48 |
| 3.318 | 10 | 211 | 26.85 |
| 2.870 | 30 | 220 | 31.14 |
| 2.447 | 75 | 311 | 36.69 |
| 2.344 | 45 | 222 | 38.37 |
| 2.170 | <1 | 321 | 41.59 |
| 2.031 | 12 | 400 | 44.58 |
| 1.970 | <1 | 410 | 46.04 |

| $d (\text{\AA})$ | I | hkl | $2^\circ (\text{ })$ |
|------------------|-----|--------|----------------------|
| 1.914 | 1 | 330 | 47.46 |
| 1.863 | 20 | 331 | 48.85 |
| 1.816 | 17 | 420 | 50.19 |
| 1.772 | 1 | 421 | 51.53 |
| 1.732 | 1 | 332 | 52.82 |
| 1.658 | 13 | 422 | 55.37 |
| 1.5923 | <1 | 510 | 57.86 |
| 1.5626 | 11 | 333 | 59.07 |
| 1.5079 | 1 | 432 | 61.44 |
| 1.4827 | <1 | 521 | 62.60 |
| 1.4352 | 8 | 440 | 64.92 |
| 1.3919 | 1 | 530 | 67.20 |
| 1.3723 | 15 | 531 | 68.29 |
| 1.3532 | 7 | 600 | 69.39 |
| 1.3348 | 1 | 610 | 70.49 |
| 1.3171 | 1 | 611 | 71.58 |
| 1.2836 | 3 | 620 | 73.75 |
| 1.2681 | <1 | 621 | 74.81 |
| 1.2380 | 5 | 533 | 76.95 |
| 1.2237 | 5 | 622 | 78.02 |
| 1.2103 | <1 | 630 | 79.05 |
| 1.1719 | 2 | 444 | 82.19 |
| 1.1367 | 5 | 551 | 85.32 |
| 1.1259 | 2 | 640 | 86.34 |
| 1.1151 | 1 | 720 | 87.38 |
| 1.0848 | 4 | 642 | 90.48 |
| 1.0570 | 5 | 731 | 93.56 |
| 1.0149 | <1 | 800 | 98.75 |
| 1.0071 | <1 | 740 | 99.79 |
| .9918 | 1 | 733 | 101.91 |
| .9844 | 2 | 820 | 102.98 |
| .9567 | 2 | 660 | 107.24 |
| .9375 | 3 | 751 | 110.50 |
| .9313 | 1 | 662 | 111.61 |
| .9078 | 1 | 840 | 116.11 |
| .8910 | 2 | 911 | 119.65 |
| .8857 | 1 | 842 | 120.84 |
| .8654 | 1 | 664 | 125.76 |
| .8510 | 1 | 931 | 129.69 |
| .8285 | 1 | 844 | 136.80 |
| .8158 | 2 | 755 | 141.53 |
| .8119 | 1 | 860 | 143.17 |
| .7960 | 2 | 10.2.0 | |
| .7848 | <1 | 951 | 157.94 |

References

- Birnstock, R. (1967). Z. Krist. **124**, 310.
- Swanson, H.E. and Tatge, E. (1953). Natl. Bur. Std. U.S. Circ. 539, 1, 81.

Cadmium bromide chloride, CdBrCl

Sample

The sample was prepared by melting a 1:1 molar mixture of CdBr₂ and CdCl₂. This was then annealed for three days at 300°C in a sealed tube.

Color

Light grey

Structure

Hexagonal, R̄3m (166), Z = 3, isostructural with CdCl₂. The structure of CdCl₂ was determined by Pauling [1929]. A complete solid solution exists between CdBr₂ and CdCl₂ [Nacken, 1907].

NBS lattice constants:

$$\begin{aligned} a &= 3.9204(3) \text{\AA} \\ c &= 18.408(2) \end{aligned}$$

Density
(calculated) 4.630 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 3.3$$

References

- Nacken, R. (1907). Centr. Mineral Geol. 1907, 303.
 Pauling, L. (1929). Proc. Nat. Acad. Sci. U.S. 15, 709.

| Internal standard W, a = 3.16516 Å $\text{CuK}\alpha_1 \lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|---|----------|------------|--------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2</i> (°) |
| 6.137 | 100 | 003 | 14.42 |
| 3.340 | 30 | 101 | 26.67 |
| 3.068 | 1 | 006 | 29.08 |
| 2.734 | 60 | 104 | 32.73 |
| 2.496 | 10 | 015 | 35.95 |
| 2.081 | 6 | 107 | 43.46 |
| 2.046 | 3 | 009 | 44.23 |
| 1.961 | 25 | 110 | 46.26 |
| 1.905 | 17 | 018 | 47.70 |
| 1.868 | 10 | 113 | 48.71 |
| 1.690 | 3 | 021 | 54.22 |
| 1.5928 | 7 | 024 | 57.84 |
| 1.5417 | 1 | 205 | 59.95 |
| 1.5338 | 4 | 0.0.12 | 60.29 |
| 1.5013 | 1 | 0.1.11 | 61.74 |
| 1.4268 | 1 | 027 | 65.35 |
| 1.4154 | 2 | 119 | 65.94 |
| 1.3662 | 3 | 208 | 68.64 |
| 1.3070 | <1 | 1.0.13 | 72.22 |
| 1.2801 | 2 | 211 | 73.99 |
| 1.2359 | 4 | 214 | 77.11 |
| 1.2272 | 1 | 0.0.15 | 77.76 |
| 1.2116 | 1 | 125 | 78.95 |
| 1.2079 | 4 | 1.1.12 | 79.24 |
| 1.1917 | <1 | 2.0.11 | 80.53 |
| 1.1534 | 1 | 217 | 83.80 |
| 1.1317 | 2 | 300 | 85.79 |
| 1.1206 | 2 | 128 | 86.85 |
| 1.1129 | <1 | 303 | 87.60 |
| 1.0897 | 1 | 1.0.16 | 89.96 |
| 1.0400 | <1 | 1.1.15 | 95.57 |
| 1.0315 | <1 | 0.1.17 | 96.62 |
| 1.0183 | <1 | 1.2.11 | 98.30 |

Calcium aluminum hydroxide, $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$

Sample

The sample was prepared by treating a saturated solution of CaO with 6% phenol. Aluminum metal dissolved in KOH was added. The compound was then dried at 110 °C for two hours.

Color

Colorless

Optical data

Isotropic, N = 1.605

Structure

Cubic, Ia3d (230), Z = 8, garnet type [Flint et al., 1941].

NBS lattice constant:
a = 12.5727(2) Å

Density
(calculated) 2.527 g/cm³

Reference intensity

$I/I_{\text{corundum}} = 1.0$

Additional patterns

1. PDF 3-125 [Flint et al., 1941]

References

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

| d (Å) | I | Internal standard W, $a = 3.16516$ Å | |
|---------|-----|--------------------------------------|---------------|
| | | hkl | 2γ (°) |
| 5.130 | 90 | 211 | 17.27 |
| 4.442 | 40 | 220 | 19.97 |
| 3.358 | 55 | 321 | 26.52 |
| 3.142 | 45 | 400 | 28.38 |
| 2.810 | 80 | 420 | 31.82 |
| 2.680 | 6 | 332 | 33.41 |
| 2.566 | 15 | 422 | 34.94 |
| 2.465 | 30 | 431 | 36.42 |
| 2.295 | 100 | 521 | 39.23 |
| 2.222 | 4 | 440 | 40.56 |
| 2.039 | 95 | 611 | 44.39 |
| 1.989 | 8 | 620 | 45.58 |
| 1.8536 | 1 | 631 | 49.11 |
| 1.8148 | 10 | 444 | 50.23 |
| 1.7785 | 2 | 543 | 51.33 |
| 1.7437 | 40 | 640 | 52.43 |
| 1.7111 | 20 | 721 | 53.51 |
| 1.6800 | 50 | 642 | 54.58 |
| 1.5964 | 11 | 732 | 57.70 |
| 1.5715 | 13 | 800 | 58.70 |
| 1.5478 | 1 | 741 | 59.69 |
| 1.5249 | 1 | 820 | 60.68 |
| 1.5030 | 2 | 653 | 61.66 |
| 1.4818 | 3 | 660 | 62.64 |
| 1.4616 | 1 | 831 | 63.61 |
| 1.4243 | 1 | 752 | 65.48 |
| 1.4058 | 12 | 840 | 66.45 |
| 1.3716 | 5 | 842 | 68.33 |
| 1.3555 | 5 | 761 | 69.26 |
| 1.3401 | 8 | 664 | 70.17 |
| 1.3253 | 2 | 851 | 71.07 |
| 1.2965 | 5 | 932 | 72.90 |
| 1.2835 | 2 | 844 | 73.76 |
| 1.2701 | 4 | 941 | 74.67 |
| 1.2449 | 2 | 10.1.1 | 76.45 |
| 1.2330 | 1 | 10.2.0 | 77.32 |
| 1.2216 | 1 | 943 | 78.18 |
| 1.1986 | 8 | 10.3.1 | 79.98 |
| 1.1774 | <1 | 871 | 81.72 |
| 1.1673 | 8 | 10.4.0 | 82.58 |
| 1.1574 | 4 | 10.3.3 | 83.45 |
| 1.1478 | 10 | 10.4.2 | 84.30 |
| 1.1382 | 1 | 873 | 85.18 |
| 1.1202 | 8 | 11.2.1 | 86.89 |
| 1.1113 | 4 | 880 | 87.76 |

Calcium aluminum hydroxide, $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$ — continued

| d (\AA) | I | hkl | $2\cdot$ ($^\circ$) |
|----------------------|-----|--------|-----------------------|
| 1.0863 | 4 | 11·3·2 | 90.32 |
| 1.0624 | 1 | 10·6·2 | 92.94 |
| 1.0551 | 2 | 965 | 93.78 |
| 1.0478 | 2 | 12·0·0 | 94.64 |
| 1.0406 | 1 | 11·4·3 | 95.50 |
| 1.0337 | 2 | 12·2·0 | 96.35 |
| 1.0266 | 2 | 11·5·2 | 97.24 |
| 1.0197 | 5 | 12·2·2 | 98.12 |
| 1.0132 | 1 | 12·3·1 | 98.97 |
| 0.9758 | 5 | 11·6·3 | 104.26 |
| .9532 | 2 | 13·2·1 | 107.83 |
| .9477 | 1 | 12·4·4 | 108.74 |
| .9371 | 5 | 12·6·0 | 110.56 |
| .9320 | 3 | 13·3·2 | 111.47 |
| .9268 | 3 | 12·6·2 | 112.43 |
| .9220 | 1 | 13·4·1 | 113.33 |
| .9073 | 1 | 888 | 116.19 |
| .8935 | 1 | 13·5·2 | 119.11 |
| .8890 | 1 | 14·2·0 | 120.09 |
| .8846 | 1 | 12·7·3 | 121.10 |
| .8760 | 3 | 14·3·1 | 123.13 |
| .8718 | 2 | 12·8·0 | 124.15 |
| .8675 | <1 | 13·5·4 | 125.23 |
| .8635 | 3 | 14·4·0 | 126.26 |
| .8593 | <1 | 14·3·3 | 127.38 |
| .8554 | 8 | 14·4·2 | 128.44 |

Calcium chloride (hydrophilite), CaCl_2

Sample

CaCO_3 was slowly converted to CaCl_2 by exposure to dry HCl fumes. However, since a few peaks of another phase persisted in the sample it was felt that intensity values should be calculated rather than measured.

Color

Colorless

Structure

Orthorhombic, Pnnm (58), $Z=2$, distorted rutile arrangement. The structure was determined by van Bever and Nieuwenkamp [1935]. Intensity values were calculated from structure data using the following information:

NBS lattice constants:

$$a = 6.261(2)\text{\AA}$$

$$b = 6.429(2)$$

$$c = 4.167(1)$$

Atom positions:

Ca (0 0 0)
Cl (.275 .325 0) [van Bever and Nieuwenkamp, 1935]

Scattering factors:

Ca^{2+} , Cl^- [International Tables, 1962]

Thermal parameters:

$$\text{overall } B = 1.0$$

Density

(calculated) 2.175 g/cm³

Polymorphism

Jensen [1943] described 3 modifications.

| Internal standard W, $a = 3.16516 \text{\AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|--|----------------|-------|----------------------|
| $d (\text{\AA})$ | I (calc.) | hkl | $2\theta (\text{°})$ |
| 4.48 | 85 | 110 | 19.80 |
| 3.46 | 17 | 101 | 25.71 |
| 3.050 | 100 | 111 | 29.26 |
| 2.858 | 35 | 120 | 31.27 |
| 2.816 | 4 | 210 | 31.75 |
| 2.356 | 25 | 121 | 38.16 |
| 2.331 | 50 | 211 | 38.59 |
| 2.244 | 30 | 220 | 40.16 |
| 2.083 | 20 | 002 | 43.40 |
| 2.027 | 3 | 130 | 44.66 |
| 1.974 | 2 | 221 | 45.94 |
| 1.906 | 25 | 031 | 47.68 |
| 1.890 | 10 | 112 | 48.10 |
| 1.866 | 11 | 301 | 48.75 |
| 1.792 | 10 | 311 | 50.92 |
| 1.751 | 4 | 320 | 52.20 |
| 1.684 | 7 | 122 | 54.44 |
| 1.565 | 4 | 400 | 58.97 |
| 1.527 | 10 | 222 | 60.59 |
| 1.496 | 4 | 330 | 62.00 |

Additional patterns

1. PDF card 1-0338 [Hanawalt et al., 1938]
2. Döll and Klemm [1939]

References

- van Bever, A. K. and Nieuwenkamp, W. (1935). Z. Krist. 90, 374.
- Döll, W. and Klemm, W. (1939). Z. anorg. u. allgem. Chem. 241, 233.
- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938) Ind. Eng. Chem. Anal. Ed. 10, 457.
- International Tables III (1962). 202, 204.
- Jensen, A.T. (1943). Kgl. Danske Videnskab. Selskab 20 #5, 1.

Cesium cobalt chloride, Cs_2CoCl_4

Sample

The sample was prepared by slow evaporation at room temperature of a 2:1 aqueous solution of CsCl and CoCl_2 .

Color

Brilliant greenish blue

Optical data

Biaxial, $N_\alpha = 1.575$, $N_\beta = 1.585$, $N_\gamma = 1.596$; $2V$ is very large.

Structure

Orthorhombic, Pnam (62), $Z=4$, isostructural with K_2SO_4 and Cs_2CuCl_4 [Porai-Koshitz, 1954]. The structure was determined by Tishchenko and Pinsker [1955].

NBS lattice constants:

$$a = 9.771(2) \text{\AA}$$

$$b = 12.973(2)$$

$$c = 7.401(1)$$

Density

(calculated) 3.303 g/cm^3

Reference intensity

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

Major impurities

$\sim .05\%$ Al, Cu, Si, and Zn.

References

Porai-Koshitz, M.A. (1954). Tr. Inst. Kristallogr. Akad. Nauk SSSR **10**, 269.

Tishchenko, G.N. and Pinsker, Z.G. (1955). Dokl. Akad. Nauk SSSR **100**, 913.

| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
|------------------|-----|------------|---------------------------|
| 2.904 | 40 | 311 | 30.76 |
| 2.875 | 55 | 212 | 31.08 |
| 2.841 | 30 | 141 | 31.46 |
| 2.700 | 35 | 240, 132 | 33.15 |
| 2.684 | 30 | 222 | 33.36 |
| 2.600 | 40 | 330 | 34.46 |
| 2.537 | 8 | 241 | 35.35 |
| 2.507 | 12 | 150 | 35.78 |
| 2.447 | 20 | 051 | 36.70 |
| 2.436 | 40 | 232 | 36.87 |
| 2.402 | 20 | 312, 410 | 37.41 |
| 2.319 | 5 | 401 | 38.80 |
| 2.297 | 8 | 340 | 39.18 |
| 2.284 | 16 | 411 | 39.42 |
| 2.245 | 13 | 123 | 40.14 |
| 2.194 | 19 | 341 | 41.11 |
| 2.170 | 10 | 213 | 41.59 |
| 2.142 | 13 | 033 | 42.16 |
| 2.126 | 9 | 332, 430 | 42.48 |
| 2.093 | 2 | 133 | 43.18 |
| 2.086 | 4 | 223 | 43.35 |
| 2.076 | 11 | 152 | 43.57 |
| 1.976 | 6 | 260 | 45.88 |
| 1.951 | 11 | 342, 440 | 46.50 |
| 1.945 | 13 | 422, 313 | 46.66 |
| 1.925 | 6 | 143 | 47.17 |
| 1.910 | 5 | 261 | 47.56 |
| 1.870 | 13 | 520, 511 | 48.65 |
| 1.850 | 16 | 004 | 49.21 |
| 1.843 | 13 | 432 | 49.40 |
| 1.822 | 3 | 243, 170 | 50.03 |
| 1.798 | 10 | 071 | 50.74 |
| 1.779 | 5 | 352, 024 + | 51.30 |
| 1.750 | 5 | 124, 361 | 52.24 |
| 1.744 | 14 | 262 | 52.41 |
| 1.730 | 6 | 531, 204 | 52.88 |
| 1.714 | 7 | 512 | 53.42 |
| 1.687 | 3 | 271 | 54.32 |
| 1.682 | 8 | 343 | 54.50 |
| 1.670 | 18 | 522 | 54.93 |
| 1.632 | 9 | 541 | 56.31 |
| 1.629 | 8 | 600 | 56.45 |
| 1.622 | 3 | 080 | 56.69 |
| 1.6068 | 11 | 044 | 57.29 |
| 1.6037 | 9 | 163, 452 | 57.41 |
| 1.6004 | 10 | 180 | 57.54 |
| 1.5969 | 9 | 314 | 57.68 |
| 1.5911 | 7 | 601 | 57.91 |
| 1.5858 | 4 | 144 | 58.12 |
| 1.5431 | 2 | 263 | 59.89 |
| 1.5276 | 7 | 551 | 60.56 |
| 1.5081 | 6 | 334 | 61.43 |
| 1.4891 | 5 | 154 | 62.30 |

Cesium copper chloride, Cs_2CuCl_4

Sample

The sample was prepared by slow evaporation at room temperature of a 2:1 molar aqueous solution of CsCl and CuCl_2 .

Color

Unground - deep brown
Ground - deep orange

Optical data

Biaxial (+), $N_\alpha = 1.625$, $N_\beta = 1.648$, $N_\gamma = 1.678$
 $2V = 83^\circ 46'$ [Helmholz and Kruh, 1952].

Structure

Orthorhombic, Pnam (62), $Z = 4$. The space group was determined by Mellor [1939]. The structure was determined by Helmholz and Kruh [1952], and refined by Morosin and Lingafelter [1961].

NBS lattice constants:

$$\begin{aligned} a &= 9.773(2)\text{\AA} \\ b &= 12.415(2) \\ c &= 7.617(2) \end{aligned}$$

Density
(calculated) 3.386 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 1.2$$

References

- Helmholz, L. and Kruh, R.F. (1952). J. Am. Chem. Soc. **74**, 1176.
 Mellor, D.P. (1939). Z. Krist. **101A**, 160.
 Morosin, B. and Lingafelter, E.C. (1961). J. Phys. Chem. **65**, 50.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ \text{ C}$ | | | |
|--|-----|---------|---------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 5.236 | 2 | 120 | 16.92 |
| 4.546 | 11 | 210 | 19.51 |
| 4.316 | 55 | 121 | 20.56 |
| 4.116 | 25 | 201 | 21.57 |
| 3.905 | 40 | 211 | 22.75 |
| 3.841 | 35 | 220 | 23.14 |
| 3.808 | 100 | 130,002 | 23.34 |
| 3.638 | 50 | 031 | 24.45 |
| 3.410 | 5 | 112,131 | 26.11 |
| 3.247 | 2 | 022 | 27.45 |
| 3.157 | 60 | 230 | 28.24 |
| 3.152 | 60 | 310 | 28.29 |
| 3.103 | 60 | 040 | 28.75 |
| 3.082 | 30 | 122 | 28.95 |
| 3.005 | 16 | 202 | 29.71 |
| 2.959 | 4 | 140 | 30.18 |
| 2.920 | 25 | 212,231 | 30.59 |
| 2.913 | 25 | 311 | 30.67 |
| 2.884 | 25 | 320 | 30.98 |
| 2.758 | 16 | 141 | 32.43 |
| 2.704 | 25 | 222 | 33.10 |
| 2.696 | 25 | 321,132 | 33.20 |
| 2.560 | 30 | 330 | 35.02 |
| 2.477 | 12 | 241 | 36.23 |
| 2.442 | 9 | 400 | 36.77 |
| 2.429 | 35 | 232,312 | 36.97 |
| 2.406 | 25 | 150,042 | 37.35 |
| 2.361 | 3 | 051 | 38.09 |
| 2.300 | 7 | 322 | 39.14 |
| 2.286 | 20 | 411,123 | 39.38 |
| 2.274 | 6 | 420 | 39.60 |
| 2.253 | 5 | 203 | 39.99 |
| 2.247 | 3 | 340 | 40.09 |
| 2.217 | 12 | 213 | 40.67 |
| 2.179 | 2 | 421 | 41.40 |
| 2.164 | 11 | 033 | 41.71 |
| 2.156 | 13 | 242,341 | 41.87 |
| 2.124 | 10 | 251,332 | 42.53 |
| 2.056 | 2 | 402 | 44.00 |
| 2.033 | 11 | 152 | 44.52 |
| 2.028 | 10 | 412,431 | 44.64 |
| 1.980 | 5 | 233 | 45.79 |
| 1.977 | 3 | 313,350 | 45.86 |
| 1.953 | 3 | 422 | 46.47 |
| 1.935 | 5 | 342 | 46.92 |
| 1.929 | 7 | 510,143 | 47.06 |
| 1.910 | 8 | 351 | 47.56 |
| 1.904 | 25 | 260,004 | 47.72 |
| 1.872 | 5 | 511 | 48.60 |
| 1.864 | 7 | 520 | 48.82 |

Cesium copper chloride, Cs_2CuCl_4 – continued

| d (\AA) | I | hkl | 2β ($^\circ$) |
|----------------------|-----|---------|-----------------------|
| 1.848 | 2 | 261,114 | 49.26 |
| 1.842 | 4 | 432 | 49.45 |
| 1.823 | 3 | 243 | 49.99 |
| 1.819 | 4 | 062 | 50.12 |
| 1.788 | 4 | 124,162 | 51.04 |
| 1.7673 | 3 | 530 | 51.68 |
| 1.7562 | 2 | 214 | 52.03 |
| 1.7428 | 5 | 413 | 52.46 |
| 1.7269 | 14 | 071 | 52.98 |
| 1.7218 | 16 | 512,531 | 53.15 |
| 1.7031 | 17 | 262,134 | 53.78 |
| 1.6979 | 11 | 451 | 53.96 |
| 1.6826 | 4 | 343 | 54.49 |
| 1.6746 | 6 | 522 | 54.77 |
| 1.6668 | 4 | 270 | 55.05 |
| 1.6546 | 3 | 540 | 55.49 |
| 1.6298 | 12 | 314,600 | 56.41 |
| 1.6234 | 8 | 044 | 56.65 |
| 1.6169 | 9 | 541 | 56.90 |
| 1.6030 | 9 | 532 | 57.44 |
| 1.5886 | 6 | 324 | 58.01 |
| 1.5786 | 6 | 611,460 | 58.41 |
| 1.5590 | 3 | 353 | 59.22 |
| 1.5366 | 3 | 513,550 | 60.17 |
| 1.5276 | 9 | 334,272 | 60.56 |
| 1.5166 | 5 | 542 | 61.05 |

Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by evaporating an aqueous solution of CoCl_2 at about 90 °C. The first crystals formed were filtered from the solution and washed with ethyl alcohol. The sample forms a higher hydrate in moist air.

Color

Deep violet

Structure

Monoclinic, $C2/m$ (12), $Z = 2$, isostructural with $\text{CoBr}_2 \cdot 2\text{H}_2\text{O}$ and the corresponding Mn salts [Morosin, 1965]. The structure of $\text{CoBr}_2 \cdot 2\text{H}_2\text{O}$ was determined by Morosin and Graeber [1963].

NBS lattice constants:

$$a = 7.280(1)\text{\AA}$$

$$b = 8.552(2)$$

$$c = 3.573(1)$$

$$\beta = 97.55(1)^\circ$$

Density

(calculated) 2.498 g/cm^3

Reference intensity

$$I/I_{\text{CuK}\alpha_1} = 2.5$$

Additional patterns

1. PDF card 3-786 [Neuhaus, 1938].

References

Morosin, B. (1965). Abstract Bull. Am. Phys. Soc. 10, 686.

Morosin, B. and Graeber, E.J. (1963). Acta Cryst. 16, 1176.

Neuhaus, A. (1938). Z. Krist. 98, 112.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ\text{C}$ | | | |
|--|-----|----------|-------------------------|
| $d (\text{\AA})$ | I | hkl | $2\psi (\text{)}^\circ$ |
| 5.514 | 100 | 110 | 16.06 |
| 4.277 | 65 | 020 | 20.75 |
| 3.606 | 2 | 200 | 24.67 |
| 3.542 | 3 | 001 | 25.13 |
| 3.127 | 4 | 111 | 28.52 |
| 2.854 | 25 | 111 | 31.32 |
| 2.758 | 14 | 220 | 32.43 |
| 2.726 | 20 | 021 | 32.83 |
| 2.712 | 40 | 201 | 33.00 |
| 2.651 | 11 | 130 | 33.78 |
| 2.376 | 25 | 201 | 37.84 |
| 2.315 | 4 | 310 | 38.87 |
| 2.291 | 12 | 221 | 39.30 |
| 2.138 | 20 | 040 | 42.23 |
| 2.076 | 19 | 131, 221 | 43.56 |
| 2.0611 | 12 | 311 | 43.89 |
| 1.8350 | 4 | 311 | 49.64 |
| 1.8044 | 8 | 400 | 50.54 |
| 1.7711 | 6 | 002 | 51.56 |
| 1.7379 | 6 | 112 | 52.62 |
| 1.7031 | 5 | 331 | 53.78 |
| 1.6789 | 10 | 241 | 54.62 |
| 1.6626 | 6 | 420 | 55.20 |
| 1.6359 | 3 | 022 | 56.18 |
| 1.5896 | 10 | 241 | 57.97 |
| 1.4233 | 3 | 510 | 65.53 |
| 1.3938 | 1 | 350 | 67.09 |
| 1.3786 | 5 | 440 | 67.94 |

Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of CoCl_2 .

Color

Deep purplish red

Optical data

Biaxial (+), $N_\alpha = 1.524$, $N_\beta = 1.548$, $N_\gamma = 1.580$. $2V$ is very large.

Structure

Monoclinic, $I2/m$ (12), $Z = 2$, isostructural with $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$. The structure was determined by Mizuno (1960).

NBS lattice constants:

$$a = 8.898(2) \text{\AA}$$

$$b = 7.066(1)$$

$$c = 6.644(1)$$

$$\beta = 97.25(1)^\circ$$

Density (calculated) 1.907 g/cm^3

Polymorphism

1. PDF card 13-399 [Inst. of Physics, University College, Cardiff, Wales] reports a cell related to this form but with the c doubled and with space group $P2_1/c$ (14). The pattern however appears quite different, so a polymorph may exist.

References

Mizuno, J. (1960). J. Phys. Soc. Japan 15, 1412.

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}$; temp. 25° C | | | |
|---|-----|------------------|----------------------------|
| $d (\text{\AA})$ | I | hkl | $2^\circ (\text{ }^\circ)$ |
| 5.636 | 100 | $\bar{1}01$ | 15.71 |
| 5.521 | 45 | 110 | 16.04 |
| 4.987 | 15 | 101 | 17.77 |
| 4.826 | 55 | 011 | 18.37 |
| 4.421 | 4 | 200 | 20.07 |
| 3.534 | 18 | 020 | 25.18 |
| 3.414 | 4 | $\bar{2}11$ | 26.08 |
| 3.115 | 11 | 211 | 28.63 |
| 2.993 | 16 | $\bar{1}21$ | 29.83 |
| 2.933 | 55 | $\bar{1}12$ | 30.45 |
| 2.817 | 20 | $\bar{2}02$ | 31.74 |
| 2.758 | 30 | 220 | 32.44 |
| 2.735 | 16 | 112 | 32.72 |
| 2.716 | 35 | 310 | 32.95 |
| 2.569 | 19 | 301 | 34.89 |
| 2.410 | 30 | 022 | 37.28 |
| 2.219 | 10 | 031 | 40.63 |
| 2.206 | 25 | $400, \bar{3}21$ | 40.87 |
| 2.079 | 10 | $411, 321$ | 43.49 |
| 2.038 | 7 | 222 | 44.41 |
| 1.985 | 18 | 312 | 45.66 |
| 1.951 | 5 | $\bar{4}02, 231$ | 46.51 |
| 1.940 | 5 | 411 | 46.80 |
| 1.902 | 17 | $\bar{1}32$ | 47.77 |
| 1.871 | 8 | 420 | 48.62 |
| 1.8664 | 8 | $\bar{1}23$ | 48.75 |
| 1.8388 | 4 | 330 | 49.53 |
| 1.8118 | 4 | 213 | 50.32 |
| 1.7873 | 3 | 123 | 51.06 |
| 1.7666 | 7 | 040 | 51.70 |
| 1.7075 | 15 | $\bar{4}22$ | 53.63 |
| 1.6852 | 3 | $\bar{1}41$ | 54.40 |
| 1.6136 | 9 | $\bar{1}14$ | 57.03 |
| 1.6115 | 8 | $\bar{2}04$ | 57.11 |
| 1.5989 | 6 | $\bar{4}31$ | 57.60 |
| 1.5769 | 3 | $\bar{5}21$ | 58.48 |
| 1.5564 | 10 | $042, \bar{2}33$ | 59.33 |
| 1.5540 | 6 | 332 | 59.43 |
| 1.5041 | 4 | 323 | 61.61 |
| 1.4932 | 3 | 024 | 62.11 |
| 1.4837 | 3 | 204 | 62.55 |
| 1.4694 | 5 | $\bar{5}03$ | 63.23 |
| 1.4665 | 5 | $233, \bar{2}24$ | 63.37 |
| 1.4554 | 3 | 341 | 63.91 |

Cobalt fluoride hydrate, $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation of an aqueous solution of CoF_2 at room temperature.

Color
Medium red

Structure

Orthorhombic, $P2_1ab$ (29), $Z = 4$, isostructural with $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ and other similar tetrahydrates. The structure of $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ was investigated by Rao et al. [1965].

NBS lattice constants:

$$\begin{aligned}a &= 7.552(2)\text{\AA} \\b &= 12.658(3) \\c &= 5.287(1)\end{aligned}$$

Density
(calculated) 2.221 g/cm^3

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

Polymorphism

Easwaran and Srinivasan [1965] reported, by comparison of powder patterns, that $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$ was isostructural with $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$. However, Penfold and Taylor [1960] reported $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ as rhombohedral. This suggests a second form of $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$ exists.

Additional patterns

1. PDF card 1-258 [Hanawalt et al., 1938]

References

- Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.
- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
- Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. 13, 953.
- Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. 3, 68.

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|--|-----|----------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 5.289 | 5 | 001 | 16.75 |
| 4.854 | 100 | 120, 011 | 18.26 |
| 4.096 | 35 | 111 | 21.68 |
| 3.776 | 4 | 200 | 23.54 |
| 3.577 | 3 | 121 | 24.87 |
| 3.296 | 4 | 031 | 27.03 |
| 3.165 | 25 | 040 | 28.17 |
| 3.071 | 3 | 201 | 29.05 |
| 3.019 | 5 | 131 | 29.56 |
| 2.987 | 30 | 211 | 29.89 |
| 2.919 | 2 | 140 | 30.60 |
| 2.764 | 15 | 221 | 32.36 |
| 2.644 | 1 | 002 | 33.88 |
| 2.589 | 3 | 012 | 34.62 |
| 2.557 | 7 | 141 | 35.07 |
| 2.484 | 3 | 231 | 36.13 |
| 2.448 | 5 | 112 | 36.68 |
| 2.338 | 3 | 320 | 38.48 |
| 2.321 | 4 | 122 | 38.76 |
| 2.281 | 2 | 051 | 39.47 |
| 2.237 | 7 | 311 | 40.29 |
| 2.186 | 8 | 151 | 41.26 |
| 2.165 | 14 | 202 | 41.68 |
| 2.136 | 4 | 212 | 42.28 |
| 2.031 | 20 | 160 | 44.58 |
| 2.001 | 4 | 331 | 45.28 |
| 1.959 | 6 | 061, 142 | 46.31 |
| 1.954 | 7 | 251 | 46.44 |
| 1.927 | 3 | 232 | 47.12 |
| 1.889 | 6 | 400 | 48.14 |
| 1.845 | 1 | 341 | 49.34 |
| 1.8044 | 5 | 312 | 50.54 |
| 1.7869 | 8 | 242 | 51.07 |
| 1.7606 | 5 | 411 | 51.89 |
| 1.7515 | 11 | 322 | 52.18 |
| 1.7465 | 7 | 013 | 52.34 |
| 1.7117 | 2 | 421, 071 | 53.49 |
| 1.6921 | 2 | 351 | 54.16 |
| 1.6732 | 3 | 332 | 54.82 |
| 1.6696 | 3 | 171 | 54.95 |
| 1.6563 | 3 | 123 | 55.43 |
| 1.6456 | 3 | 252 | 55.82 |
| 1.6213 | 3 | 440 | 56.73 |
| 1.6169 | 3 | 360 | 56.90 |
| 1.5893 | 2 | 133 | 57.98 |

Copper fluoride hydrate, CuF₂·2H₂O

Sample

The sample was prepared by slow evaporation of a CuF₂ aqueous solution at room temperature.

Color

Brilliant greenish blue

Optical data

Biaxial (-), N _{α} =1.502, N _{β} =1.522, N _{γ} =1.534; 2V is medium large.

Structure

Monoclinic, I2/m (12), Z=2. The structure was determined by Abrahams and Prince [1962] using neutron diffraction.

NBS lattice constants:

$$a = 6.412(1)\text{\AA}$$

$$b = 7.403(1)$$

$$c = 3.3025(6)$$

$$\beta = 99.46(1)^\circ$$

Density (calculated) 2.954 g/cm³
Reference intensity

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

Additional patterns

1. PDF card 6-143 [Wheeler and Haendler, 1954].

References

Abrahams, S. C. and Prince, E. (1962). J. Chem. Phys. 36, 50.

Wheeler, C.M.Jr. and Haendler, H.M. (1954). J. Am. Chem. Soc. 76, 263.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|--|----------|------------|--------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2</i> (°) |
| 4.805 | 100 | 110 | 18.45 |
| 3.700 | 30 | 020 | 24.03 |
| 3.164 | 17 | 200 | 28.18 |
| 3.113 | 15 | 101 | 28.65 |
| 2.983 | 12 | 011 | 29.93 |
| 2.717 | 45 | 101 | 32.94 |
| 2.404 | <1 | 220 | 37.37 |
| 2.353 | 15 | 211 | 38.22 |
| 2.299 | 20 | 130 | 39.16 |
| 2.191 | 8 | 121 | 41.16 |
| 2.023 | 15 | 211 | 44.77 |
| 1.968 | 6 | 031 | 46.08 |
| 1.919 | 13 | 301 | 47.32 |
| 1.850 | 11 | 040 | 49.20 |
| 1.750 | 6 | 231 | 52.24 |
| 1.704 | 5 | 321 | 53.75 |
| 1.650 | 2 | 301 | 55.64 |
| 1.629 | <1 | 002 | 56.44 |
| 1.601 | 12 | 231 | 57.51 |
| 1.5818 | 5 | 400 | 58.28 |
| 1.5556 | 4 | 202 | 59.36 |
| 1.5299 | 6 | 141 | 60.46 |
| 1.5079 | <1 | 321 | 61.44 |
| 1.4930 | 2 | 411 | 62.12 |
| 1.4906 | <1 | 022 | 62.23 |
| 1.4544 | <1 | 420 | 63.96 |
| 1.4413 | <1 | 150 | 64.61 |
| 1.4342 | <1 | 222 | 64.97 |
| 1.3685 | 1 | 132 | 68.51 |
| 1.3598 | <1 | 202 | 69.01 |
| 1.3325 | 4 | 341 | 70.63 |

Europium phosphate, EuPO₄

Sample

The sample was made by I. Mayer [Hebrew University, Jerusalem]. A mixture of (NH₄)₂HPO₄ and Eu₂O₃ was heated at 500 °C for 2 hours, then at 1100 °C overnight.

Color

Colorless

Structure

Monoclinic, P2₁/n (14), Z=4, isostructural with monazite [Feigelson, 1964]. The structure of monazite was determined by Kokkoros [1942].

NBS lattice constants:
 a = 6.6684(5) Å
 b = 6.8671(5)
 c = 6.3534(5)
 β = 103.94(1) °

Density

(calculated) 5.808 g/cm³

Additional patterns

1. PDF card 18-506 [Bril and Wanmaker, 1964]

References

- Bril, A. and Wanmaker, W.L. (1964). J. Electrochem. Soc. 111, 1363.
 Kokkoros, P. (1942). Prakt. Akad. Anthemon 17, 163.
 Feigelson, R.S. (1964). J. Am. Ceram. Soc. 47, 257.

| Internal standard W, a = 3.16516 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C | | | |
|--|-----|----------|--------|
| d (Å) | I | hkl | 2θ (°) |
| 5.127 | 12 | 101 | 17.28 |
| 4.714 | 9 | 110 | 18.81 |
| 4.593 | 25 | 011 | 19.31 |
| 4.107 | 40 | 111 | 21.62 |
| 4.008 | 18 | 101 | 22.16 |
| 3.461 | 17 | 111 | 25.72 |
| 3.435 | 15 | 020 | 25.92 |
| 3.237 | 55 | 200 | 27.53 |
| 3.084 | 7 | 002 | 28.93 |
| 3.034 | 100 | 120 | 29.41 |
| 3.000 | 5 | 021 | 29.76 |
| 2.928 | 15 | 210 | 30.51 |
| 2.901 | 6 | 211 | 30.80 |
| 2.813 | 85 | 112, 012 | 31.79 |
| 2.561 | 25 | 202 | 35.01 |
| 2.446 | 2 | 211 | 36.71 |
| 2.399 | 18 | 212 | 37.45 |
| 2.395 | 19 | 112 | 37.52 |
| 2.355 | 6 | 220 | 38.18 |
| 2.342 | 1 | 221 | 38.41 |
| 2.296 | 5 | 122, 022 | 39.21 |
| 2.208 | 3 | 301 | 40.83 |
| 2.146 | 25 | 031 | 42.07 |
| 2.112 | 25 | 103 | 42.79 |
| 2.104 | 25 | 311 | 42.96 |
| 2.081 | 19 | 221 | 43.44 |
| 2.058 | 2 | 310 | 43.96 |
| 2.053 | 3 | 222 | 44.08 |
| 1.988 | 2 | 131 | 45.60 |
| 1.923 | 35 | 212 | 47.22 |
| 1.899 | 6 | 301 | 47.87 |
| 1.868 | 3 | 230 | 48.70 |
| 1.862 | 14 | 231 | 48.88 |
| 1.839 | 25 | 132, 032 | 49.53 |
| 1.835 | 15 | 103 | 49.64 |
| 1.827 | 15 | 320 | 49.87 |
| 1.7988 | 2 | 123 | 50.71 |
| 1.7737 | 2 | 113 | 51.48 |
| 1.7638 | 11 | 023 | 51.79 |
| 1.7339 | 19 | 322 | 52.75 |
| 1.7227 | 4 | 231 | 53.12 |
| 1.7170 | 5 | 040 | 53.31 |
| 1.7043 | 25 | 132, 223 | 53.74 |
| 1.6593 | 11 | 140 | 55.32 |
| 1.6377 | 1 | 141 | 56.49 |
| 1.6180 | 4 | 123, 400 | 56.86 |
| 1.6002 | 7 | 402 | 57.55 |
| 1.5782 | 2 | 141 | 58.43 |
| 1.5750 | 7 | 410 | 58.56 |
| 1.5701 | 7 | 330 | 58.76 |

Europium phosphate, EuPO₄ – continued

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2θ</i> (°) |
|--------------|----------|------------|---------------|
| 1.5583 | 2 | 412 | 59.25 |
| 1.5547 | 4 | 312 | 59.40 |
| 1.5476 | 2 | 114 | 59.70 |
| 1.5420 | 5 | 004 | 59.94 |
| 1.5322 | 2 | 213 | 60.36 |
| 1.5288 | 1 | 033, 323 | 60.51 |
| 1.5168 | 3 | 240 | 61.04 |
| 1.5101 | 5 | 332 | 61.34 |
| 1.5059 | 10 | 214 | 61.53 |
| 1.5003 | 4 | 142, 042 | 61.78 |
| 1.4503 | 2 | 422 | 64.16 |
| 1.4473 | 1 | 322, 411 | 64.31 |
| 1.4417 | 4 | 124 | 64.59 |
| 1.4358 | 3 | 241 | 64.89 |
| 1.4322 | 2 | 133 | 65.07 |
| 1.4295 | 3 | 223 | 65.21 |
| 1.4260 | 3 | 242 | 65.39 |
| 1.4062 | 1 | 024 | 66.43 |
| 1.3974 | 3 | 314 | 66.90 |
| 1.3591 | 2 | 421 | 69.05 |
| 1.3473 | 4 | 431 | 69.74 |
| 1.3434 | 5 | 150, 340 | 69.97 |
| 1.3379 | 3 | 423 | 70.30 |
| 1.3320 | 3 | 143 | 70.66 |
| 1.3263 | 2 | 151 | 71.01 |
| 1.3179 | 4 | 324, 043 | 71.53 |
| 1.3152 | 7 | 124 | 71.70 |
| 1.3091 | 11 | 332, 402 | 72.09 |
| 1.3052 | 10 | 342, 134 | 72.34 |

Glucose, D, alpha, (dextrose), C₆H₁₂O₆

Sample

The sample was NBS Standard Reference Material 41a. The dextrose was produced by Pfanstiehl Laboratories, Inc. Chicago, Illinois
 moisture..... less than 0.02%
 ash..... less than 0.01%

Color

Colorless

Structure

Orthorhombic, P2₁2₁2₁(19). Z=4, [Sponsler and Dove, 1931]. The structure was determined by McDonald and Beevers [1952].

NBS lattice constants:

$$\begin{aligned}a &= 10.368(2) \text{\AA} \\b &= 14.856(2) \\c &= 4.9808(6)\end{aligned}$$

Density
 (calculated) 1.560 g/cm³

Reference intensity
 $I/I_{\text{corundum}} = 2.3$

Additional patterns

1. PDF card 1-374 [Sponsler and Dove, 1931]
2. PDF card 3-228 Inst. of Physics at University College, Cardiff, Wales.

References

- McDonald, T.R.R. and Beevers, C.A. (1952). Acta Cryst. **5**, 654.
 Sponsler, O.L. and Dove, W.H. (1931). J. Am. Chem. Soc. **53**, 1639.

| Internal standard Ag, a = 4.08641 Å CuK α_1 , $\lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|--|----------|------------|---------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2θ</i> (°) |
| 8.50 | 7 | 110 | 10.40 |
| 7.42 | 6 | 020 | 11.91 |
| 6.04 | 15 | 120 | 14.66 |
| 5.181 | 14 | 200 | 17.10 |
| 4.894 | 1 | 210 | 18.11 |
| 4.724 | 20 | 011 | 18.77 |
| 4.487 | 4 | 101 | 19.77 |
| 4.298 | 100 | 111 | 20.65 |
| 4.251 | 8 | 220 | 20.88 |
| 3.841 | 4 | 121 | 23.14 |
| 3.709 | 1 | 040 | 23.97 |
| 3.590 | 4 | 201 | 24.78 |
| 3.493 | 11 | 140,211 | 25.48 |
| 3.366 | 2 | 310 | 26.46 |
| 3.326 | 3 | 131 | 26.78 |
| 3.234 | 2 | 221 | 27.56 |
| 3.132 | 19 | 320 | 28.47 |
| 3.018 | 1 | 240 | 29.57 |
| 2.977 | 2 | 041 | 29.99 |
| 2.907 | 4 | 231 | 30.73 |
| 2.856 | 4 | 150 | 31.29 |
| 2.833 | 1 | 330 | 31.55 |
| 2.789 | <1 | 311 | 32.06 |
| 2.651 | 2 | 321 | 33.78 |
| 2.590 | 5 | 400 | 34.60 |
| 2.581 | 4 | 241 | 34.73 |
| 2.551 | 4 | 410,051 | 35.15 |
| 2.530 | 2 | 340 | 35.45 |
| 2.489 | 8 | 002 | 36.05 |
| 2.477 | 9 | 151,060 | 36.23 |
| 2.455 | 7 | 012 | 36.57 |
| 2.449 | 7 | 420 | 36.67 |
| 2.423 | 2 | 102 | 37.08 |
| 2.408 | 1 | 160 | 37.31 |
| 2.390 | 1 | 112 | 37.60 |
| 2.362 | 7 | 022 | 38.07 |
| 2.295 | 4 | 430 | 39.22 |
| 2.273 | 4 | 411 | 39.62 |
| 2.255 | 6 | 341 | 39.94 |
| 2.233 | 1 | 260 | 40.35 |
| 2.217 | 4 | 061 | 40.66 |
| 2.196 | 1 | 421 | 41.06 |
| 2.168 | 1 | 161 | 41.62 |
| 2.150 | 1 | 222 | 41.99 |
| 2.125 | <1 | 440 | 42.51 |
| 2.085 | 1 | 431 | 43.36 |
| 2.080 | 1 | 170 | 43.47 |
| 2.053 | 4 | 510,351 | 44.08 |
| 2.002 | 1 | 312 | 45.26 |
| 1.963 | 2 | 270 | 46.20 |

Glucose, D, alpha, (dextrose), C₆H₁₂O₆ – continued

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2θ (°) |
|--------------|----------|------------|--------|
| 1.953 | 2 | 450,071 | 46.47 |
| 1.918 | 2 | 171 | 47.36 |
| 1.914 | 2 | 501,530 | 47.47 |
| 1.899 | 1 | 511 | 47.87 |
| 1.867 | 1 | 361 | 48.74 |
| 1.854 | 1 | 521 | 49.10 |
| 1.827 | 1 | 180,271 | 49.87 |
| 1.818 | <1 | 451 | 50.14 |
| 1.809 | <1 | 370 | 50.40 |
| 1.791 | 2 | 252,460 | 50.95 |
| 1.786 | 1 | 531 | 51.10 |
| 1.775 | <1 | 342 | 51.43 |
| 1.756 | 1 | 062 | 52.05 |
| 1.745 | <1 | 422 | 52.39 |
| 1.741 | <1 | 081 | 52.52 |
| 1.716 | <1 | 610,181 | 53.35 |
| 1.701 | 1 | 541,550+ | 53.86 |
| 1.684 | 1 | 461,620 | 54.44 |
| 1.671 | 1 | 352 | 54.90 |
| 1.663 | 1 | 262 | 55.18 |
| 1.650 | <1 | 013,281 | 55.66 |
| 1.630 | 1 | 190,113 | 56.39 |
| 1.623 | 1 | 611 | 56.65 |
| 1.617 | <1 | 442 | 56.90 |
| 1.601 | 1 | 123 | 57.53 |
| 1.595 | 2 | 172,621 | 57.75 |
| 1.5811 | 1 | 203 | 58.31 |
| 1.5664 | 1 | 091,640+ | 58.91 |

Indium sulfide, In_2S_3

Sample

The In_2S_3 was made by W.S. Brower by heating the elements in a sealed silica tube at 460 °C for sixteen hours and at 880 °C for six hours.

Color

Unground: dark grayish red
Ground: strong reddish brown

Structure

Tetragonal, I4₁22 (98), Z=16. The structure was studied by Rooymans [1959] and by Goodyear and Steigmann [1961].

NBS lattice constants:
 $a = 7.619(1)\text{\AA}$
 $c = 32.329(4)$

Density
 (calculated) 4.613 g/cm³

Reference intensity
 $I/I_{\text{corundum}} = 4.2$

Polymorphism

Hahn and Klinger [1949] found that a low temperature form transformed irreversibly at about 330 °C to a high form which they indexed as cubic with a few extra non-cubic lines.

Additional patterns

1. Goodyear and Steigmann [1961].

References

- Goodyear, J. and Steigmann, G.A. (1961). Proc. Phys. Soc. 78 491.
 Hahn, H. and Klinger, W. (1949). Z. anorg. Chem. 260, 97.
 Rooymans, C.J.M. (1959). J. Inorg. Nucl. Chem. 11, 78.

| Internal standard W, $a = 3.16516 \text{\AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{\AA}; \text{temp. } 25^\circ\text{C}$ | | | |
|---|-----|---------------|--------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (^\circ)$ |
| 8.09 | 4 | 004 | 10.93 |
| 7.40 | 3 | 101 | 11.95 |
| 6.21 | 30 | 103 | 14.24 |
| 5.110 | 12 | 112 | 17.34 |
| 4.927 | 2 | 105 | 17.99 |
| 4.041 | 3 | 008 | 21.98 |
| 3.947 | 2 | 107 | 22.51 |
| 3.811 | 18 | 200,116 | 23.32 |
| 3.445 | 2 | 204 | 25.84 |
| 3.392 | 2 | 211 | 26.25 |
| 3.249 | 100 | 109,213 | 27.43 |
| 3.112 | 12 | 206 | 28.66 |
| 3.015 | 1 | 215 | 29.60 |
| 2.770 | 3 | 208,1·1·10 | 32.29 |
| 2.741 | 3 | 1·0·11,217 | 32.64 |
| 2.694 | 50 | 0·0·12,220 | 33.23 |
| 2.557 | 1 | 224 | 35.07 |
| 2.532 | 1 | 301 | 35.42 |
| 2.472 | 4 | 219,303 | 36.31 |
| 2.382 | 1 | 312 | 37.74 |
| 2.364 | 3 | 1·0·13,305 | 38.04 |
| 2.309 | 1 | 314 | 38.97 |
| 2.225 | 3 | 2·1·11,307 | 40.51 |
| 2.199 | 9 | 2·0·12,316 | 41.00 |
| 2.123 | 1 | 1·1·14 | 42.54 |
| 2.107 | 2 | 321 | 42.88 |
| 2.074 | 45 | 309,323 | 43.61 |
| 2.009 | 3 | 2·1·13,325 | 45.09 |
| 1.905 | 65 | 2·2·12,400 | 47.71 |
| 1.845 | 1 | 1·0·17,411 | 49.34 |
| 1.8213 | 6 | 329,413,+ | 50.04 |
| 1.7766 | 1 | 3·0·13,415 | 51.39 |
| 1.7224 | 1 | 334,408,+ | 53.13 |
| 1.7161 | 1 | 3·2·11,417 | 53.34 |
| 1.7037 | 3 | 336,420,+ | 53.76 |
| 1.6673 | 3 | 3·1·14,424 | 55.03 |
| 1.6615 | 3 | 1·0·19,2·1·17 | 55.24 |
| 1.6429 | 13 | 3·0·15,419 | 55.92 |
| 1.6242 | 5 | 426,2·0·18 | 56.62 |
| 1.6161 | 3 | 2·2·16,0·0·20 | 56.93 |
| 1.5701 | 2 | 3·3·10,428 | 58.76 |
| 1.5647 | 2 | 4·1·11 | 58.98 |
| 1.5556 | 10 | 4·0·12 | 59.36 |
| 1.5224 | 1 | 2·1·19,431,+ | 60.79 |
| 1.5090 | 4 | 1·0·21,3·2·15 | 61.39 |
| 1.4876 | 3 | 2·0·20,512 | 62.37 |
| 1.4835 | 2 | 4·1·13,435 | 62.56 |
| 1.4475 | 1 | 437 | 64.30 |
| 1.4403 | 4 | 3·1·18,516,+ | 64.66 |
| 1.4181 | 2 | 1·1·22,3·3·14 | 65.80 |

Indium sulfide, In_2S_3 – continued

| d (\AA) | I | hkl | 2ϕ ($^\circ$) |
|----------------------|-----|---------------|----------------------|
| 1.4137 | 2 | 3·0·19,521,+ | 66.03 |
| 1.4028 | 16 | 439,523,+ | 66.61 |
| 1.3527 | 2 | 4·3·11,527 | 69.42 |
| 1.3470 | 8 | 440,0·0·24 | 69.76 |
| 1.3252 | 1 | 3·2·19,4·1·17 | 71.08 |
| 1.2746 | 1 | 1·0·25,5·2·11 | 74.36 |
| 1.2701 | 2 | 2·0·24,536,+ | 74.67 |
| 1.2442 | 9 | 4·3·15,613,+ | 76.50 |
| 1.2364 | 2 | 4·2·18,606 | 77.07 |
| 1.2301 | 2 | 3·0·23,615,+ | 77.54 |
| 1.2119 | 1 | 1·1·26,608,+ | 78.93 |
| 1.2046 | 6 | 4·4·12,620,+ | 79.49 |
| 1.1895 | 1 | 4·3·17,541 | 80.72 |
| 1.1829 | 1 | 1·0·27,619,+ | 81.26 |
| 1.1728 | 1 | 4·2·20 | 82.11 |
| 1.1524 | 1 | 3·0·25,547,+ | 83.89 |
| 1.1488 | 1 | 5·1·18,6·0·12 | 84.21 |
| 1.1294 | 5 | 549,633,+ | 86.00 |
| 1.1190 | 1 | 4·1·23,635,+ | 87.00 |
| 1.0997 | 14 | 4·0·24,6·2·12 | 88.93 |
| 1.0832 | <1 | 3·0·27,639,+ | 90.65 |
| 1.0566 | 2 | 556,640,+ | 93.61 |
| 1.0462 | 2 | 6·1·17,721 | 94.83 |
| 1.0418 | 7 | 3·2·27,709,+ | 95.36 |
| 1.0368 | 4 | 6·0·18,646,+ | 95.97 |
| 1.0334 | 3 | 1·0·31,725,+ | 96.38 |
| 1.0223 | 1 | 5·5·10,648,+ | 97.79 |
| 1.0048 | 1 | 6·3·15,729 | 100.10 |
| 0.9715 | 2 | 7·0·15,653,+ | 104.91 |
| .9524 | 4 | 4·4·24,800 | 107.96 |
| .9413 | 1 | 659,743,+ | 109.83 |

Iron chloride hydrate, $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by permitting anhydrous FeCl_2 to hydrate in humid air. The sample was somewhat hygroscopic.

Color

light yellowish brown

Structure

Monoclinic, $C2/m$ (12), $Z=2$, isostructural with $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$ and $\text{MnCl}_2 \cdot 2\text{H}_2\text{O}$. The structure was determined by Morosin and Graeber [1965].

NBS lattice constants: .

$$a = 7.3523(6)\text{\AA}$$

$$b = 8.5609(8)$$

$$c = 3.6367(3)$$

$$\beta = 98.10(1)^\circ$$

Density

(calculated) 2.385 g/cm^3

Additional patterns

- PDF card 1-210 [Hanawalt et al., 1938]

References

- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938).
Ind. Eng. Chem. Anal. Ed. **10**, 457.
Morosin, B. and Graeber, E. J. (1965). J. Chem. Phys. **42**, 898.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
|---|-----|-------|-------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
| 5.548 | 100 | 110 | 15.96 |
| 4.281 | 75 | 020 | 20.73 |
| 3.641 | 7 | 200 | 24.43 |
| 3.600 | 7 | 001 | 24.71 |
| 3.181 | 8 | 111 | 28.03 |
| 2.884 | 45 | 111 | 30.98 |
| 2.773 | 45 | 220 | 32.25 |
| 2.763 | 90 | 201 | 32.38 |
| 2.657 | 25 | 130 | 33.70 |
| 2.396 | 45 | 201 | 37.50 |

| $d (\text{\AA})$ | I | hkl | $2\theta (\circ)$ |
|------------------|-----|----------|-------------------|
| 2.335 | 12 | 310 | 38.53 |
| 2.321 | 25 | 221 | 38.77 |
| 2.193 | 5 | 131 | 41.13 |
| 2.141 | 35 | 040 | 42.18 |
| 2.092 | 45 | 311, 221 | 43.21 |
| 2.088 | 35 | 131 | 43.30 |
| 1.848 | 7 | 330, 311 | 49.26 |
| 1.840 | 6 | 041 | 49.51 |
| 1.820 | 19 | 400 | 50.09 |
| 1.800 | 13 | 002 | 50.67 |
| 1.769 | 14 | 112 | 51.62 |
| 1.721 | 9 | 331 | 53.18 |
| 1.711 | 7 | 202 | 53.49 |
| 1.692 | 20 | 241 | 54.17 |
| 1.674 | 11 | 420 | 54.79 |
| 1.6668 | 9 | 150 | 55.05 |
| 1.6609 | 8 | 112 | 55.26 |
| 1.6593 | 7 | 022 | 55.32 |
| 1.5959 | 18 | 241 | 57.72 |
| 1.5772 | 4 | 331 | 58.47 |
| 1.5313 | 4 | 151 | 60.40 |
| 1.5270 | 7 | 132 | 60.59 |
| 1.4943 | 6 | 151 | 62.06 |
| 1.4485 | 3 | 421 | 64.25 |
| 1.4352 | 4 | 510 | 64.92 |
| 1.4268 | 5 | 060 | 65.35 |
| 1.3987 | 3 | 350 | 66.83 |
| 1.3863 | 9 | 440 | 67.51 |
| 1.3775 | 8 | 042 | 68.00 |
| 1.3408 | 6 | 351, 312 | 70.13 |
| 1.3263 | <4 | 061 | 71.01 |
| 1.3138 | <4 | 422 | 71.79 |
| 1.2966 | <4 | 530 | 72.89 |
| 1.2739 | <4 | 511 | 74.41 |
| 1.2693 | <4 | 351 | 74.72 |
| 1.2677 | 4 | 261 | 74.83 |
| 1.2432 | 4 | 152 | 76.57 |
| 1.2254 | 4 | 261, 332 | 77.89 |
| 1.2065 | 4 | 512, 170 | 79.35 |
| 1.2021 | 4 | 601 | 79.70 |
| 1.1981 | 4 | 402 | 80.02 |
| 1.1906 | <4 | 203 | 80.63 |
| 1.1741 | <4 | 531 | 82.00 |
| 1.1605 | 4 | 442 | 83.17 |
| 1.1572 | 4 | 621 | 83.46 |
| 1.1536 | 4 | 422 | 83.78 |
| 1.1481 | 4 | 113 | 84.28 |
| 1.1472 | 4 | 223 | 84.36 |
| 1.1357 | <4 | 171 | 85.41 |
| 1.1317 | <4 | 313 | 85.78 |

Lead bromide chloride, PbBrCl

Sample

The sample was prepared by melting a 1:1 mixture of PbCl₂ and PbBr₂. The sample was then ground and annealed in a sealed glass tube at 400 °C overnight.

Color

Colorless

Structure

Orthorhombic, Pnam (62), Z=4, isostructural with BaCl₂. There is a complete solid solution series between PbBr₂ and PbCl₂ [Calingaert et al., 1949]. The structure of PbCl₂ was determined by Bräkken and Harang [1928].

NBS lattice constants:

$$a = 7.801(1) \text{ \AA}$$

$$b = 9.207(1)$$

$$c = 4.5803(5)$$

Density

(calculated) 6.512 g/cm³

Reference intensity

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

References

Bräkken, H. and Harang, L. (1928). Z. Krist. 68, 123.

Calingaert, G., Lamb, F.W., and Meyers, F. (1949). J. Am. Chem. Soc. 71, 3712.

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|---|-----|----------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 5.949 | 2 | 110 | 14.88 |
| 4.607 | 6 | 020 | 19.25 |
| 4.101 | 17 | 011 | 21.65 |
| 3.964 | 80 | 120 | 22.41 |
| 3.897 | 30 | 200 | 22.80 |
| 3.632 | 90 | 111 | 24.49 |
| 2.998 | 30 | 121 | 29.78 |
| 2.976 | 20 | 220 | 30.00 |
| 2.856 | 16 | 130 | 31.29 |
| 2.826 | 100 | 211 | 31.64 |
| 2.550 | 50 | 031 | 35.17 |
| 2.503 | 8 | 310 | 35.84 |
| 2.496 | 3 | 221 | 35.95 |
| 2.423 | 16 | 131 | 37.07 |
| 2.302 | 40 | 040 | 39.09 |
| 2.291 | 40 | 002 | 39.30 |
| 2.264 | 40 | 320 | 39.78 |
| 2.207 | 10 | 140 | 40.85 |
| 2.196 | 40 | 311 | 41.06 |
| 2.134 | 40 | 231 | 42.32 |
| 2.051 | 1 | 022 | 44.12 |
| 2.030 | 1 | 321 | 44.61 |
| 1.982 | 30 | 122, 240 | 45.74 |
| 1.949 | 10 | 400 | 46.55 |
| 1.908 | 1 | 410 | 47.63 |
| 1.821 | 1 | 331, 241 | 50.05 |
| 1.815 | 5 | 222 | 50.22 |
| 1.795 | 1 | 420, 401 | 50.83 |
| 1.7922 | 3 | 150 | 50.91 |
| 1.7869 | 4 | 132 | 51.07 |
| 1.7616 | 2 | 411 | 51.86 |
| 1.7239 | 1 | 340 | 53.08 |
| 1.7090 | 1 | 051 | 53.58 |
| 1.6895 | 3 | 312 | 54.25 |
| 1.6682 | 16 | 151 | 55.00 |
| 1.6229 | 10 | 042 | 56.67 |
| 1.6102 | 20 | 322 | 57.16 |
| 1.5896 | 3 | 142 | 57.97 |
| 1.5647 | 3 | 251 | 58.98 |
| 1.5488 | 7 | 431 | 59.65 |
| 1.5348 | 2 | 060 | 60.25 |
| 1.5052 | 8 | 013, 160 | 61.56 |
| 1.4984 | 6 | 332, 242 | 61.87 |
| 1.4874 | 6 | 440 | 62.38 |
| 1.4846 | 10 | 402 | 62.51 |
| 1.4786 | 9 | 113 | 62.79 |
| 1.4663 | 1 | 412 | 63.38 |
| 1.4581 | 12 | 511 | 63.78 |
| 1.4278 | 16 | 260, 351 | 65.30 |
| 1.4245 | 4 | 123 | 65.47 |

Lead bromide chloride, PbBrCl - continued

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2θ (°) |
|--------------|----------|------------|---------------|
| 1.4111 | 1 | 152 | 66.17 |
| 1.4052 | 8 | 213 | 66.48 |
| 1.3770 | 1 | 342 | 68.03 |
| 1.3672 | 6 | 033 | 68.58 |
| 1.3463 | 2 | 252,133 | 69.80 |
| 1.3310 | 4 | 531 | 70.72 |
| 1.3216 | 1 | 360 | 71.30 |
| 1.3030 | 4 | 313 | 72.48 |
| 1.2900 | 5 | 233 | 73.33 |
| 1.2751 | 1 | 062 | 74.33 |
| 1.2639 | 5 | 071 | 75.10 |
| 1.2580 | 3 | 162 | 75.51 |
| 1.2479 | 3 | 171,442 | 76.23 |
| 1.2416 | 4 | 522 | 76.69 |
| 1.2395 | 3 | 611 | 76.84 |
| 1.2119 | 6 | 262 | 78.93 |
| 1.2025 | 2 | 271,403 | 79.67 |
| 1.1920 | 1 | 413 | 80.51 |
| 1.1626 | 3 | 153 | 82.99 |
| 1.1586 | 2 | 631 | 83.34 |

Magnesium bromide hydrate, $MgBr_2 \cdot 6H_2O$

Sample

The sample was prepared by treating $MgCO_3$ with a slight excess of an aqueous solution of HBr and evaporating at about 80 °C. The first crystals formed were used.

Color

Colorless

Structure

Monoclinic, C2/m (12), $Z = 2$, isostructural with $MgCl_2 \cdot 6H_2O$. The structure was determined by Andress and Gundermann [1934].

NBS lattice constants:

$$a = 10.286(1) \text{ \AA}$$

$$b = 7.331(1)$$

$$c = 6.211(1)$$

$$\beta = 93.34(1)^\circ$$

Density

(calculated) 2.076 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 2.9$$

Additional patterns

1. PDF card 1-1045 [Hanawalt et al., 1938].

| Internal standard W, $a = 3.16516 \text{ \AA}$ $CuK\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|---|-----|---------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 6.20 | 10 | 001 | 14.28 |
| 5.133 | 5 | 200 | 17.26 |
| 4.375 | 2 | 111 | 20.28 |
| 4.225 | 100 | 111 | 21.01 |
| 4.070 | 40 | 201 | 21.82 |
| 3.844 | 2 | 201 | 23.12 |
| 3.664 | 35 | 020 | 24.27 |
| 3.154 | 10 | 021 | 28.27 |
| 3.101 | 40 | 310,002 | 28.77 |
| 2.982 | 30 | 220 | 29.94 |
| 2.835 | 18 | 311 | 31.53 |
| 2.791 | 30 | 112 | 32.04 |
| 2.724 | 70 | 202,221 | 32.85 |
| 2.717 | 55 | 311,112 | 32.94 |
| 2.655 | 3 | 221 | 33.73 |
| 2.589 | 1 | 202 | 34.62 |
| 2.568 | 1 | 400 | 34.91 |
| 2.423 | 5 | 401 | 37.08 |
| 2.378 | 6 | 130 | 37.80 |
| 2.368 | 7 | 022 | 37.97 |
| 2.325 | 14 | 401 | 38.70 |
| 2.254 | 1 | 312 | 39.97 |
| 2.210 | 9 | 131 | 40.79 |
| 2.187 | 1 | 222 | 41.25 |
| 2.136 | 4 | 312 | 42.27 |
| 2.114 | 6 | 222 | 42.73 |
| 2.067 | 1 | 003 | 43.77 |
| 2.037 | 3 | 402 | 44.44 |
| 2.021 | 3 | 421 | 44.80 |
| 1.989 | 4 | 330 | 45.58 |
| 1.973 | 4 | 13 | 45.95 |
| 1.963 | 4 | 421 | 46.20 |
| 1.958 | 4 | 203 | 46.34 |
| 1.933 | 2 | 113 | 46.98 |
| 1.915 | 8 | 511 | 47.43 |
| 1.899 | 12 | 132 | 47.86 |
| 1.879 | 6 | 203 | 48.39 |
| 1.875 | 10 | 331,132 | 48.51 |
| 1.8543 | 2 | 511 | 49.09 |
| 1.8329 | 4 | 040 | 49.70 |
| 1.8004 | 2 | 023 | 50.66 |
| 1.7804 | 7 | 422 | 51.27 |
| 1.7634 | 4 | 313 | 51.80 |
| 1.7266 | 3 | 223,240 | 52.99 |
| 1.7117 | 3 | 600,512 | 53.49 |
| 1.7034 | 2 | 422 | 53.77 |
| 1.6792 | 3 | 313 | 54.61 |
| 1.6718 | 6 | 223,241 | 54.87 |
| 1.6576 | 2 | 403 | 55.38 |
| 1.6486 | 2 | 332 | 55.71 |

Magnesium bromide hydrate, $\text{MgBr}_2 \cdot 6\text{H}_2\text{O}$ – continued

| <i>d</i> (\AA) | <i>I</i> | <i>hkl</i> | 2θ ($^\circ$) |
|---------------------------|----------|-----------------|------------------------|
| 1.6261 | 2 | 512,601 | 56.55 |
| 1.5720 | 2 | 530 | 58.68 |
| 1.5667 | 2 | 403 | 58.90 |
| 1.5504 | 5 | 620,004 | 59.58 |
| 1.5403 | 5 | 531 | 60.01 |
| 1.5213 | 2 | $\bar{2}42$ | 60.84 |
| 1.5128 | 4 | T14 | 61.22 |
| 1.5085 | 3 | $\bar{2}04,531$ | 61.41 |
| 1.4958 | 1 | 242 | 61.99 |
| 1.4861 | 2 | 621 | 62.44 |
| 1.4609 | 2 | $\bar{4}41,204$ | 63.64 |
| 1.4581 | 2 | 333 | 63.78 |
| 1.4391 | 4 | 441 | 64.72 |
| 1.4280 | 2 | $\bar{5}32,024$ | 65.29 |
| 1.4189 | 2 | 711 | 65.76 |
| 1.4156 | 1 | T51 | 65.93 |
| 1.4103 | 2 | 151 | 66.21 |
| 1.3906 | 1 | 513 | 67.27 |
| 1.3776 | <1 | 532 | 67.99 |
| 1.3625 | 2 | $\bar{4}04,442$ | 68.85 |
| 1.3573 | 3 | $\bar{6}03,224$ | 69.15 |
| 1.3475 | 2 | 350 | 69.73 |
| 1.3381 | 1 | $\bar{2}43$ | 70.29 |
| 1.3341 | 2 | 712 | 70.53 |
| 1.3231 | 1 | 351 | 71.21 |
| 1.3189 | <1 | T52 | 71.47 |
| 1.3120 | 2 | 243 | 71.90 |
| 1.3106 | 1 | 351,152 | 71.99 |

Magnesium chloride hydrate (bischofite), $MgCl_2 \cdot 6H_2O$

Sample

The sample was prepared by boiling a saturated aqueous solution of $MgCl_2$ and filtering off the crystals. The sample was somewhat hygroscopic.

Color

Colorless

Optical data

Biaxial (+), $N_\alpha = 1.498$, $N_\beta = 1.505$, $N_\gamma = 1.525$. $2V$ is large.

Structure

Monoclinic, C2/m (12), $Z = 2$, isostructural with $MgBr_2 \cdot 6H_2O$. The structure of bischofite was determined by Andress and Gundermann [1934].

NBS lattice constants:

$a = 9.871(2)\text{\AA}$
 $b = 7.113(1)$
 $c = 6.079(1)$
 $\beta = 93.74(1)$

Density

(calculated) 1.585 g/cm^3

Reference intensity

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

Additional patterns

1. PDF card 1-431 [Hanawalt et al., 1938].

References

Andress, K.R. and Gundermann, J. (1934). Z. Krist. 87A, 345.

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

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $CuK\alpha_1, \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ \text{ C}$ | | | |
|--|-----|----------|---------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 5.77 | 17 | 110 | 15.34 |
| 4.263 | 20 | 111 | 20.82 |
| 4.101 | 100 | 111 | 21.65 |
| 3.955 | 30 | 201 | 22.46 |
| 3.708 | 10 | 201 | 23.98 |
| 3.556 | 30 | 020 | 25.02 |
| 3.068 | 2 | 021 | 29.08 |
| 3.032 | 5 | 002 | 29.43 |
| 2.981 | 35 | 310 | 29.95 |
| 2.883 | 65 | 220 | 30.99 |
| 2.740 | 35 | 311 | 32.66 |
| 2.728 | 55 | 112 | 32.80 |
| 2.661 | 8 | 202 | 33.65 |
| 2.643 | 90 | 221, 112 | 33.89 |
| 2.616 | 7 | 311 | 34.25 |
| 2.567 | 9 | 221 | 34.92 |
| 2.463 | 7 | 400 | 36.45 |
| 2.336 | 9 | 401 | 38.50 |
| 2.308 | 25 | 022, 130 | 38.99 |
| 2.232 | 30 | 401 | 40.38 |
| 2.192 | 2 | 312 | 41.15 |
| 2.167 | 5 | 131 | 41.65 |
| 2.145 | 8 | 131 | 42.10 |
| 2.131 | 3 | 222 | 42.39 |
| 2.065 | 8 | 312 | 43.80 |
| 2.051 | 11 | 222 | 44.11 |
| 1.952 | 2 | 421 | 46.49 |
| 1.922 | 5 | 330 | 47.25 |
| 1.914 | 7 | 203 | 47.46 |
| 1.890 | 6 | 421 | 48.10 |
| 1.849 | 35 | 132 | 49.25 |
| 1.844 | 20 | 511 | 49.38 |
| 1.830 | 6 | 203 | 49.79 |
| 1.812 | 7 | 331 | 50.32 |
| 1.778 | 15 | 040 | 51.35 |
| 1.757 | 5 | 023 | 52.00 |
| 1.7272 | 13 | 422 | 52.97 |
| 1.7218 | 11 | 313 | 53.15 |
| 1.6860 | 4 | 223 | 54.37 |
| 1.6418 | 3 | 600 | 55.96 |
| 1.6221 | 6 | 241 | 56.70 |
| 1.5964 | 5 | 332 | 57.70 |
| 1.5088 | 4 | 133 | 61.40 |
| 1.4874 | 12 | 531 | 62.38 |

Manganese chloride hydrate, $\text{MnCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by heating a solution of $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ in ethyl alcohol. Excess alcohol was removed by pressing between filter papers.

Color

Light pink

Optical data

Biaxial (+), $N_{\alpha} = 1.583$, $N_{\beta} = 1.613$, $N_{\gamma} = 1.664$; $2V$ is very large.

Structure

Monoclinic, $C2/m$ (12), $Z=2$ [Neuhaus, 1937], isostructural with $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$. The structure was determined by Vainshtein [1952].

NBS lattice constants:

$$\begin{aligned}a &= 7.4062(5) \text{\AA} \\b &= 8.8032(5) \\c &= 3.6881(5) \\&\beta = 98.22(1)^\circ\end{aligned}$$

Density

(calculated) 2.259 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{CuK}\alpha_1}} = 2.3$$

Additional patterns

1. PDF card 1-199 [Hanawalt et al., 1938].
2. PDF card 3-743 [Neuhaus, 1937].

References

- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.
Neuhaus, A. (1937). Z. Krist. **98**, 112.
Vainshtein, B.K. (1952). Dokl. Akad. Nauk SSSR **83**, 227.

| Internal standard W, $a = 3.16516 \text{ \AA}$ | | | |
|---|-----|----------|---------------------------|
| $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 5.636 | 100 | 110 | 15.71 |
| 4.399 | 65 | 020 | 20.17 |
| 3.667 | 3 | 200 | 24.25 |
| 3.227 | 4 | 111 | 27.62 |
| 2.922 | 25 | 111 | 30.57 |
| 2.817 | 30 | 220 | 31.74 |
| 2.794 | 45 | 201 | 32.01 |
| 2.725 | 14 | 130 | 32.84 |
| 2.419 | 25 | 201 | 37.13 |
| 2.355 | 16 | 221, 310 | 38.19 |

| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
|------------------|-----|----------|---------------------------|
| 2.202 | 19 | 040 | 40.96 |
| 2.130 | 13 | 131 | 42.41 |
| 2.120 | 20 | 221 | 42.61 |
| 2.116 | 18 | 311 | 42.70 |
| 1.887 | 1 | 240 | 48.19 |
| 1.878 | 2 | 330 | 48.43 |
| 1.866 | 2 | 311 | 48.75 |
| 1.833 | 9 | 400 | 49.71 |
| 1.8250 | 8 | 002 | 49.92 |
| 1.7945 | 7 | 112 | 50.84 |
| 1.7499 | 4 | 331 | 52.23 |
| 1.7287 | 9 | 241 | 52.92 |
| 1.7120 | 2 | 150 | 53.48 |
| 1.6918 | 5 | 420 | 54.17 |
| 1.6282 | 9 | 241 | 56.48 |
| 1.6004 | <1 | 331 | 57.54 |
| 1.5547 | 3 | 132 | 59.40 |
| 1.5304 | 2 | 151 | 60.44 |
| 1.4673 | 1 | 060 | 63.33 |
| 1.4463 | 1 | 510 | 64.36 |
| 1.4285 | 1 | 350 | 65.25 |
| 1.4084 | 6 | 440 | 66.31 |
| 1.3695 | 2 | 351 | 68.45 |
| 1.3618 | 1 | 260, 061 | 68.89 |
| 1.3116 | <1 | 530 | 71.93 |
| 1.2988 | 1 | 261 | 72.75 |
| 1.2841 | 1 | 511 | 73.72 |
| 1.2545 | 1 | 261 | 75.76 |
| 1.2393 | 1 | 170 | 76.86 |
| 1.2118 | 1 | 601 | 78.94 |
| 1.2096 | 1 | 402 | 79.11 |
| 1.1867 | <1 | 531 | 80.95 |
| 1.1771 | 1 | 620 | 81.75 |
| 1.1682 | 3 | 621 | 82.50 |
| 1.1654 | 2 | 171 | 82.75 |
| 1.1453 | 2 | 460 | 84.53 |
| 1.1363 | 1 | 532 | 85.36 |
| 1.1266 | <1 | 550 | 86.27 |
| 1.1181 | 1 | 370 | 87.09 |
| 1.1116 | 1 | 601, 551 | 87.73 |
| 1.1002 | <1 | 080 | 88.87 |
| 1.0893 | 1 | 371 | 90.00 |
| 1.0777 | <1 | 621 | 91.24 |
| 1.0658 | 1 | 461 | 92.56 |
| 1.0615 | 1 | 641 | 93.05 |
| 1.0396 | <1 | 710, 711 | 95.62 |
| 1.0372 | 1 | 172 | 95.92 |
| 1.0239 | <1 | 281 | 97.58 |
| 1.0096 | 1 | 552 | 99.45 |
| 0.9923 | 1 | 641 | 101.84 |
| 0.9862 | <1 | 730, 731 | 102.71 |

Mercury ammine chloride, $\text{Hg}(\text{NH}_3)_2\text{Cl}_2$

Sample

The sample was prepared by exposing finely ground HgCl_2 to NH_3 gas in a previously evacuated desiccator.

Color

Colorless

Structure

Cubic, $Z=1/2$, structure determined by MacGillavry and Bijvoet [1936].

NBS lattice constant:
 $a = 4.053(2)\text{\AA}$

Density
 (calculated) 3.809 g/cm^3

Reference intensity
 $I/I_{\text{corundum}} = 1.6$

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
|---|-----|-------|---------------------------|
| $d (\text{\AA})$ | I | hkl | $2^\circ (\text{)}^\circ$ |
| 2.868 | 17 | 110 | 31.16 |
| 2.342 | 100 | 111 | 38.41 |
| 2.028 | 70 | 200 | 44.65 |
| 1.4332 | 25 | 220 | 65.02 |
| 1.2220 | 19 | 311 | 78.15 |
| 1.1699 | 8 | 222 | 82.36 |

Additional patterns

- MacGillavry and Bijvoet [1936]

References

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

Neodymium phosphate, NdPO₄

Sample

The sample was made by I. Mayer [Hebrew University, Jerusalem]. A mixture of (NH₄)₂HPO₄ and Nd₂O₃ was heated at 500 °C for 2 hours, then at 1100 °C overnight.

Color

Pale purplish pink

Structure

Monoclinic, P2₁/n (14), Z=4, isostructural with monazite. The structure of NdPO₄ was determined by Mooney [1948].

NBS lattice constants:

$$\begin{aligned}a &= 6.7441(6) \text{\AA} \\b &= 6.9584(7) \\c &= 6.4111(7) \\&\beta = 103.67(1)^\circ\end{aligned}$$

Density
(calculated) 5.435 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 1.0$$

Polymorphism

NdPO₄ occurs also in a low temperature modification, which may require some zeolite water for stabilization [Mooney, 1950]. PDF card 4-644 is of this form.

Additional patterns

1. Weigel et al. [1965]

References

- Mooney, R.C.L. (1948). J. Chem. Phys. 16, 1003.
- Mooney, R.C.L. (1950). Acta Cryst. 3, 337.
- Weigel, von F., Sherer, V. and Henschel, H. (1965). Radiochimica Acta 4, 18.

| Internal standard W, a = 3.16516 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C | | | |
|--|----------|------------|--------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2</i> (°) |
| 5.17 | 14 | 101 | 17.13 |
| 4.78 | 10 | 110 | 18.56 |
| 4.645 | 25 | 011 | 19.09 |
| 4.151 | 45 | 111 | 21.39 |
| 4.064 | 16 | 101 | 21.85 |
| 3.508 | 19 | 111 | 25.37 |
| 3.479 | 18 | 020 | 25.58 |
| 3.277 | 60 | 200 | 27.19 |
| 3.116 | 8 | 002 | 28.62 |
| 3.072 | 100 | 120 | 29.04 |
| 3.040 | 7 | 021 | 29.36 |
| 2.965 | 17 | 210 | 30.12 |
| 2.933 | 5 | 211 | 30.45 |
| 2.842 | 100 | 012, 112 | 31.45 |
| 2.583 | 25 | 202 | 34.70 |
| 2.479 | <1 | 211 | 36.21 |
| 2.423 | 25 | 112, 212 | 37.08 |
| 2.385 | 7 | 220 | 37.68 |
| 2.368 | 2 | 221 | 37.97 |
| 2.321 | 6 | 022, 122 | 38.77 |
| 2.233 | 3 | 301 | 40.36 |
| 2.187 | 3 | 130 | 41.24 |
| 2.174 | 25 | 031 | 41.51 |
| 2.129 | 40 | 103 | 42.43 |
| 2.126 | 40 | 311 | 42.48 |
| 2.109 | 25 | 221 | 42.84 |
| 2.085 | 3 | 310 | 43.36 |
| 2.075 | 3 | 122, 222 | 43.58 |
| 2.038 | 1 | 113 | 44.42 |
| 2.015 | 2 | 131 | 44.95 |
| 1.991 | <1 | 013 | 45.53 |
| 1.949 | 35 | 212 | 46.55 |
| 1.924 | 9 | 301 | 47.19 |
| 1.892 | 1 | 230 | 48.04 |
| 1.885 | 16 | 231 | 48.25 |
| 1.860 | 35 | 032, 132 | 48.93 |
| 1.851 | 19 | 320 | 49.19 |
| 1.8165 | 2 | 123 | 50.18 |
| 1.7945 | 2 | 113 | 50.84 |
| 1.7834 | 11 | 023 | 51.18 |
| 1.7521 | 20 | 322 | 52.16 |
| 1.7400 | 7 | 040 | 52.55 |
| 1.7266 | 25 | 132, 232 | 52.99 |
| 1.7215 | 20 | 303 | 53.16 |
| 1.6812 | 12 | 140 | 54.54 |
| 1.6715 | 1 | 313 | 54.88 |
| 1.6494 | 1 | 141 | 55.68 |
| 1.6383 | 6 | 123, 400 | 56.09 |
| 1.6159 | 9 | 402 | 56.94 |
| 1.5989 | 2 | 141 | 57.60 |

Neodymium phosphate, NdPO₄ – continued

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2 <i>θ</i> (°) |
|--------------|----------|-------------|----------------|
| 1.5949 | 9 | 410 | 57.76 |
| 1.5903 | 8 | 330 | 57.94 |
| 1.5757 | 5 | 312 | 58.53 |
| 1.5616 | 3 | 114 | 59.11 |
| 1.5573 | 6 | 004, 204 | 59.29 |
| 1.5427 | <1 | 323 | 59.91 |
| 1.5364 | 3 | 240 | 60.18 |
| 1.5267 | 6 | 332 | 60.60 |
| 1.5193 | 13 | 214, 042 | 60.93 |
| 1.4820 | <1 | 420 | 62.63 |
| 1.4659 | 3 | 411, 422 | 63.40 |
| 1.4554 | 6 | 124, 241 | 63.91 |
| 1.4477 | 4 | 223 | 64.29 |
| 1.4431 | 4 | 142, 242 | 64.52 |
| 1.4214 | 1 | 024, 224 | 65.63 |
| 1.4092 | 3 | 314 | 66.27 |
| 1.3768 | 4 | 421 | 68.04 |
| 1.3636 | 5 | 431 | 68.79 |
| 1.3605 | 5 | 150, 340 | 68.97 |
| 1.3534 | 2 | 303 | 69.38 |
| 1.3507 | 3 | 423 | 69.54 |
| 1.3470 | 3 | 143 | 69.76 |
| 1.3436 | 3 | 151 | 69.96 |
| 1.3332 | 5 | 043 | 70.59 |
| 1.3292 | 11 | 324, 313 | 70.83 |
| 1.3270 | 13 | 332, 402 | 70.97 |
| 1.3237 | 6 | 511 | 71.17 |
| 1.3200 | 8 | 342 | 71.40 |
| 1.3187 | 8 | 134 | 71.48 |
| 1.3125 | 2 | 233 | 71.87 |
| 1.3063 | 2 | 243 | 72.27 |
| 1.3030 | 5 | 412 | 72.48 |
| 1.2927 | 5 | 034, 234, + | 73.15 |
| 1.2880 | 3 | 510 | 73.46 |
| 1.2805 | 2 | 250, 105 | 73.96 |
| 1.2701 | 12 | 152, 414, + | 74.67 |
| 1.2595 | 4 | 115, 431 | 75.41 |
| 1.2495 | 2 | 503 | 76.12 |
| 1.2382 | 6 | 522 | 76.94 |
| 1.2300 | <1 | 513 | 77.55 |
| 1.2254 | 8 | 501, 152 | 77.89 |
| 1.2228 | 12 | 334 | 78.09 |
| 1.2123 | 2 | 224 | 78.90 |

Nickel chloride hydrate, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation at room temperature of an aqueous solution of NiCl_2 (Fisher Scientific Co.). Because of the platy nature and the instability of the material, the intensity values are subject to some error.

Color

Deep yellowish green

Optical data

Biaxial (+) $N_\alpha = 1.590$, $N_\beta = 1.620$, $N_\gamma = 1.648$; $2V$ is very large.

Structure

Monoclinic, $I2/m$ (12), $Z = 2$, isostructural with $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$. The structure was determined by Mizuno (1961).

NBS lattice constants:

$a = 8.786(2)\text{\AA}$
 $b = 7.076(2)$
 $c = 6.625(2)$
 $\beta = 97.21(1)^\circ$

Density

(calculated) 1.932 g/cm^3

Additional patterns

1. PDF card 1-200 [Hanawalt et al., 1938]

References

Hanawalt, J.D., Rinn, R.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. **10**, 457.
 Mizuno, J. (1961). J. Phys. Soc. Japan **16**, 1574.

| $d (\text{\AA})$ | I | Internal standard Ag, $a = 4.08641 \text{ \AA}$ | |
|------------------|-----|---|--------------------|
| | | hkl | $2\theta (^\circ)$ |
| 5.59 | 100 | 101 | 15.83 |
| 5.50 | 40 | 110 | 16.10 |
| 4.96 | 12 | 101 | 17.88 |
| 4.82 | 35 | 011 | 18.39 |
| 4.360 | 2 | 200 | 20.35 |
| 3.542 | 10 | 020 | 25.12 |
| 3.392 | 2 | 211 | 26.25 |
| 3.288 | 1 | 002 | 27.10 |
| 3.095 | 4 | 211 | 28.82 |
| 2.994 | 9 | 121 | 29.82 |
| 2.926 | 35 | 112 | 30.53 |
| 2.799 | 17 | 202 | 31.95 |
| 2.747 | 30 | 220 | 32.57 |
| 2.729 | 5 | 112 | 32.79 |
| 2.689 | 20 | 310 | 33.29 |
| 2.543 | 8 | 301 | 35.27 |
| 2.407 | 16 | 022 | 37.32 |
| 2.220 | 3 | 031 | 40.60 |
| 2.211 | 2 | 312 | 40.77 |
| 2.192 | 5 | 103, 321 | 41.14 |
| 2.178 | 20 | 400 | 41.42 |
| 2.065 | 3 | 103, 321 | 43.81 |
| 2.057 | 7 | 411 | 43.98 |
| 2.030 | 4 | 222 | 44.59 |
| 2.013 | 1 | 231 | 45.00 |
| 1.980 | 3 | 213 | 45.80 |
| 1.971 | 8 | 312 | 46.00 |
| 1.932 | 3 | 402 | 47.00 |
| 1.921 | 3 | 411 | 47.29 |
| 1.900 | 10 | 132 | 47.83 |
| 1.862 | 5 | 123 | 48.85 |
| 1.856 | 5 | 420 | 49.03 |
| 1.832 | 2 | 330 | 49.74 |
| 1.783 | 1 | 123 | 51.20 |
| 1.695 | 7 | 422 | 54.07 |
| 1.687 | 3 | 141 | 54.35 |
| 1.636 | 1 | 501 | 56.17 |
| 1.6084 | 3 | 114, 413 | 57.23 |
| 1.6045 | 6 | 204, 033 | 57.38 |
| 1.5888 | 3 | 431 | 58.00 |
| 1.5853 | 3 | 512 | 58.14 |
| 1.5609 | 2 | 521 | 59.14 |
| 1.5575 | 2 | 042 | 59.28 |
| 1.5483 | 4 | 332 | 59.67 |
| 1.4969 | 2 | 323 | 61.94 |
| 1.4774 | 1 | 204 | 62.85 |
| 1.4628 | 2 | 233, 224 | 63.55 |
| 1.4558 | 2 | 503 | 63.89 |
| 1.4514 | 2 | 341 | 64.11 |

Nickel fluoride hydrate, $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$

Sample

The sample was made by slow evaporation at room temperature of an aqueous solution of NiF_2 with a slight excess of HF.

Color

Brilliant yellow green

Structure

Orthorhombic, $P2_1ab$ (29), $Z=4$, isostructural with $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$. The space group and cell parameters of $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ were determined by Rao et al. [1965].

NBS lattice constants:

$$a = 7.485(2)\text{\AA}$$

$$b = 12.482(2)$$

$$c = 5.272(1)$$

Density

(calculated) 2.276 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} 2.0$$

Polymorphism

Easwaran and Srinivasan [1965] reported, by comparison of powder patterns, that $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$ was isostructural with $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$. However, Penfold and Taylor [1960] reported $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ as rhombohedral. This suggests a second form of $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$ exists.

Additional patterns

1. PDF card 1-267 [Hanawalt et al., 1938]

References

- Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.
- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
- Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. 13, 953.
- Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. 3, 68.

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
|---|-----|----------|---------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 5.28 | 6 | 001 | 16.78 |
| 4.857 | 85 | 011 | 18.25 |
| 4.795 | 100 | 120 | 18.49 |
| 4.075 | 50 | 111 | 21.79 |
| 3.748 | 6 | 200 | 23.73 |
| 3.546 | 3 | 121 | 25.09 |
| 3.266 | 3 | 031 | 27.28 |
| 3.120 | 30 | 040 | 28.59 |
| 3.052 | 4 | 201 | 29.24 |
| 2.964 | 35 | 211 | 30.13 |
| 2.741 | 15 | 221 | 32.64 |
| 2.637 | 1 | 002 | 33.97 |
| 2.580 | 3 | 012 | 34.74 |
| 2.528 | 8 | 141 | 35.48 |
| 2.460 | 3 | 231 | 36.49 |
| 2.439 | 6 | 112 | 36.82 |
| 2.309 | 4 | 122 | 38.98 |
| 2.256 | 1 | 051 | 39.93 |
| 2.219 | 8 | 311 | 40.62 |
| 2.155 | 25 | 202 | 41.89 |
| 2.124 | 4 | 212 | 42.53 |
| 2.037 | 1 | 222 | 44.43 |
| 2.004 | 13 | 160 | 45.22 |
| 1.982 | 3 | 331 | 45.74 |
| 1.933 | 9 | 251 | 46.98 |
| 1.913 | 3 | 232 | 47.49 |
| 1.871 | 5 | 400 | 48.61 |
| 1.828 | 1 | 341 | 49.85 |
| 1.793 | 5 | 312, 420 | 50.90 |
| 1.773 | 10 | 242 | 51.51 |
| 1.740 | 13 | 013, 322 | 52.56 |
| 1.719 | 1 | 261 | 53.24 |
| 1.689 | 2 | 071 | 54.25 |
| 1.674 | 1 | 351 | 54.81 |
| 1.661 | 2 | 332 | 55.25 |
| 1.648 | 4 | 171 | 55.72 |
| 1.6311 | 3 | 252 | 56.36 |
| 1.6050 | 2 | 440 | 57.36 |
| 1.5974 | 3 | 360 | 57.66 |
| 1.5951 | 2 | 162 | 57.75 |
| 1.5821 | 2 | 133 | 58.27 |
| 1.5787 | 1 | 213 | 58.41 |
| 1.5607 | 1 | 080 | 59.15 |

Potassium bromide iodide, KBr_{.33}I_{.67}

Sample

The sample was prepared by melting a 1:2 mixture of KBr and KI. After grinding, it was annealed at 450 °C overnight.

Color

Colorless

Optical data

Isotropic, N=1.633

Structure

Cubic, Fm3m (225), Z = 4, NaCl type. There is a complete solid solution series from KBr to KI [Wrzesnewsky, 1912].

NBS lattice constant:

$$a = 6.9174(3)\text{\AA}$$

Density

(calculated) 3.02 g/cm³

Reference intensity

I/I_{conundum} = 8.4

References

Wrzesnewsky, J.B. (1912). Z. anorg. Chem. 74, 110.

| Internal standard Ag, a = 4.08641 Å $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|---|-----|-----|--------|
| d (Å) | I | hkl | 2θ (°) |
| 3.997 | 25 | 111 | 22.22 |
| 3.456 | 100 | 200 | 25.76 |
| 2.446 | 40 | 220 | 36.71 |
| 2.086 | 10 | 311 | 43.35 |
| 1.997 | 10 | 222 | 45.37 |
| 1.7290 | 7 | 400 | 52.91 |
| 1.5868 | 2 | 331 | 58.08 |
| 1.5464 | 10 | 420 | 59.75 |
| 1.4118 | 5 | 422 | 66.13 |
| 1.3312 | 1 | 511 | 70.71 |
| 1.2227 | 1 | 440 | 78.10 |
| 1.1694 | 1 | 531 | 82.40 |
| 1.1528 | 2 | 600 | 83.85 |
| 1.0935 | 1 | 620 | 89.56 |
| 1.0549 | <1 | 533 | 93.81 |
| 1.0428 | <1 | 622 | 95.24 |
| .9985 | <1 | 444 | 100.96 |
| .9687 | <1 | 711 | 105.34 |
| .9592 | <1 | 640 | 106.85 |
| .9245 | <1 | 642 | 112.85 |
| .9006 | <1 | 731 | 117.58 |
| .8388 | <1 | 800 | 133.34 |

Potassium bromide iodide, KBr_{.67}I_{.33}

Sample

The sample was prepared by melting together KBr and KI in a 2:1 molar ratio. After grinding the sample was heated at 400 °C overnight.

Color

Colorless

Structure

Cubic, Fm3m (225), z = 4, NaCl type. There is a complete solid solution series between KBr and KI [Wrzesnewsky, 1912].

NBS lattice constant:
a = 6.7624(3) Å

Density
(calculated) 2.90 g/cm³

Reference intensity

I/I_{corundum} = 8.4.

Optical data

Isotropic, N=1.597

| Internal standard W, a = 3.16516 Å CuKα ₁ , λ = 1.54056 Å; temp. 25 °C | | | |
|--|-----|-----|--------------------|
| d (Å) | I | hkl | 2 ^o (°) |
| 3.909 | 15 | 111 | 22.73 |
| 3.380 | 100 | 200 | 26.35 |
| 2.390 | 30 | 220 | 37.60 |
| 2.040 | 5 | 311 | 44.38 |
| 1.952 | 7 | 222 | 46.48 |
| 1.691 | 5 | 400 | 54.19 |
| 1.5514 | 2 | 331 | 59.54 |
| 1.5125 | 7 | 420 | 61.23 |
| 1.3805 | 3 | 422 | 67.83 |
| 1.3014 | 1 | 511 | 72.58 |
| 1.1959 | 1 | 440 | 80.20 |
| 1.1431 | <1 | 531 | 84.73 |
| 1.1273 | 1 | 600 | 86.20 |
| 1.0693 | 1 | 620 | 92.17 |
| 1.0193 | <1 | 622 | 98.17 |
| .9760 | <1 | 444 | 104.22 |
| .9467 | <1 | 711 | 108.90 |
| .9377 | <1 | 640 | 110.46 |
| .9036 | <1 | 642 | 116.97 |
| .8805 | <1 | 731 | 122.04 |
| .8453 | <1 | 800 | 131.36 |
| .8200 | <1 | 820 | 139.88 |

References

Wrzesnewsky, J.B. (1912). Z. anorg. Chem. 74, 110.

Potassium cobalt fluoride, K_2CoF_4

Sample

The sample was prepared by treating a 1:1 mixture of K_2CO_3 and $CoCO_3$ with HF, drying, and heating the product for 10 minutes at 400 °C, followed by 10 minutes at 750 °C.

Color

Medium pink

Structure

Tetragonal, $I4/mmm$ (139), $Z=2$, isostructural with K_2MgF_4 and similar tetrafluorides [Rüdorff et al., 1959]. The structure of K_2MgF_4 was determined by Brehler and Winkler [1954].

NBS lattice constants:

$$a = 4.0750(4)\text{\AA}$$

$$c = 13.089(1)$$

Density (calculated) 3.256 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 3.4$$

Major impurities

~ .05% Ag, Ca, Cu, Fe, Ni, Zn and Si.

~ .5% Al

References

- Brehler, B. and Winkler, H.G.F. (1954). Heidelberger Beitr. Mineral. Petrogr. 4, 6.
 Rüdorff, W., Kändler, J., Lincke, G., and Babel, D. (1959). Angew. Chem. 71, 672.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $CuK\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|---|-----|--------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 6.53 | 100 | 002 | 13.54 |
| 3.890 | 8 | 101 | 22.84 |
| 3.272 | 1 | 004 | 27.23 |
| 2.976 | 40 | 103 | 30.00 |
| 2.879 | 30 | 110 | 31.04 |
| 2.637 | 2 | 112 | 33.97 |
| 2.202 | 10 | 105 | 40.95 |
| 2.181 | 40 | 006 | 41.36 |
| 2.163 | 10 | 114 | 41.72 |
| 2.038 | 25 | 200 | 44.42 |
| 1.946 | 3 | 202 | 46.64 |
| 1.806 | 1 | 211 | 50.49 |
| 1.7394 | 7 | 116 | 52.57 |
| 1.6814 | 8 | 213 | 54.53 |
| 1.6364 | 5 | 008 | 56.16 |
| 1.4956 | 3 | 215 | 62.00 |
| 1.4891 | 9 | 206 | 62.30 |
| 1.4403 | 4 | 220 | 64.66 |
| 1.4229 | 1 | 118 | 65.55 |
| 1.3697 | 1 | 109 | 68.44 |
| 1.3089 | <1 | 000·10 | 72.10 |
| 1.2970 | 1 | 303 | 72.87 |
| 1.2884 | 2 | 310 | 73.43 |
| 1.2756 | 2 | 208 | 74.29 |
| 1.2058 | 1 | 305 | 79.41 |
| 1.2022 | 2 | 226 | 79.69 |
| 1.1919 | 1 | 1·1·10 | 80.52 |
| 1.1421 | 1 | 1·0·11 | 84.82 |
| 1.1365 | 1 | 219 | 85.34 |
| 1.1097 | 1 | 316 | 87.92 |

Potassium tungsten oxide, K_2WO_4

Sample

The sample was prepared by adding KOH solution to an aqueous solution of H_2WO_4 .

Color

Colorless

Structure

Monoclinic, C2/m (12), $Z = 4$. The structure was determined by Koster et al. (1969).

NBS lattice constants:

$$\begin{aligned}a &= 12.383(1) \text{ \AA} \\b &= 6.1194(8) \\c &= 7.5526(9) \\&\beta = 115.95(1)^\circ\end{aligned}$$

Density

(calculated) 4.208 g/cm^3

Polymorphism

K_2WO_4 undergoes a transition at 370°C [Schmitz-Dumont and Weeg, 1951]

Additional patterns

1. PDF card 19-1004 [Gelsing et al., 1965]
2. PDF card 21-703 [Hatterer et al., 1968]
3. Kools et al. [1970]

References

- Gelsing, R. J. H., Stein, H. N., and Stevels, J.M. (1965). Rec. Trav. Chim. **84**, 1452.
 Hatterer, A., Kessler, H., and Ringenbach, C. (1968). Compt. Rend. Paris **266C**, 328.
 Kools, F. X. N. M., Koster, A. S., and Rieck, G.D. (1970). Acta Cryst. **B26**, 1974.
 Koster, A.S., Kools, F. X. N. M., and Rieck, G.D. (1969). Acta Cryst. **B25**, 1704.
 Schmitz-Dumont, O. and Weeg, A. (1951). Z. Anorg. Chem. **265**, 139.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $CuK\alpha_1, \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ\text{C}$ | | | |
|---|-----|----------|------------------|
| $d (\text{\AA})$ | I | hkl | $2\cdot (\circ)$ |
| 6.80 | 8 | 001 | 13.00 |
| 5.70 | 50 | 201 | 15.52 |
| 5.566 | 30 | 200 | 15.91 |
| 5.365 | 30 | 110 | 16.51 |
| 4.719 | 90 | 111 | 18.79 |
| 3.834 | 45 | 111 | 23.18 |
| 3.708 | 25 | 202 | 23.98 |
| 3.601 | 25 | 201 | 24.70 |
| 3.397 | 85 | 002 | 26.21 |
| 3.173 | 100 | 310 | 28.10 |
| 3.092 | 19 | 401 | 28.85 |
| 3.059 | 60 | 020 | 29.17 |
| 2.928 | 60 | 312 | 30.51 |
| 2.848 | 4 | 402 | 31.38 |
| 2.784 | 14 | 400 | 32.12 |
| 2.696 | 9 | 221 | 33.20 |
| 2.683 | 7 | 220 | 33.37 |
| 2.630 | 6 | 112 | 34.06 |
| 2.359 | 6 | 222 | 38.11 |
| 2.332 | 13 | 221 | 38.57 |
| 2.324 | 9 | 403 | 38.71 |
| 2.293 | 17 | 313 | 39.26 |
| 2.273 | 45 | 022 | 39.62 |
| 2.253 | 12 | 401 | 39.98 |
| 2.240 | 11 | 512 | 40.22 |
| 2.176 | 5 | 421 | 41.46 |
| 2.092 | 3 | 510 | 43.22 |
| 2.048 | 11 | 602 | 44.18 |
| 2.030 | 4 | 601 | 44.59 |
| 2.006 | 2 | 130 | 45.17 |
| 1.978 | 25 | 312 | 45.83 |
| 1.967 | 10 | 131 | 46.10 |
| 1.944 | 5 | 113, 223 | 46.69 |
| 1.899 | 6 | 603 | 47.85 |
| 1.885 | 5 | 131 | 48.25 |
| 1.868 | 4 | 204 | 48.71 |
| 1.855 | 11 | 600, 404 | 49.07 |
| 1.849 | 12 | 423 | 49.23 |
| 1.835 | 2 | 203 | 49.63 |
| 1.814 | 8 | 421 | 50.26 |
| 1.804 | 16 | 314 | 50.56 |
| 1.788 | 14 | 330 | 51.04 |
| 1.740 | 9 | 332 | 52.55 |
| 1.706 | 11 | 514 | 53.69 |
| 1.702 | 13 | 622 | 53.82 |

Potassium tungsten oxide, K_2WO_4 – continued

| <i>d</i> (\AA) | <i>I</i> | <i>hkl</i> | 2° ($^\circ$) |
|---------------------------|----------|-----------------------|------------------------|
| 1.6984 | 10 | $\bar{7}12,004$ | 53.94 |
| 1.6671 | 3 | $\bar{6}04$ | 55.04 |
| 1.6607 | 6 | $\bar{7}11$ | 55.27 |
| 1.6351 | 3 | $\bar{7}13$ | 56.21 |
| 1.6133 | 3 | $\bar{6}23$ | 57.04 |
| | | | |
| 1.5946 | 6 | $\bar{2}24$ | 57.77 |
| 1.5866 | 9 | $620,\bar{4}24$ | 58.09 |
| 1.5742 | 6 | $223,\bar{3}33$ | 58.59 |
| 1.5559 | 4 | $\bar{5}32$ | 59.35 |
| 1.5514 | 4 | 422 | 59.54 |
| | | | |
| 1.5474 | 3 | $\bar{8}02$ | 59.71 |
| 1.5293 | 7 | $040,114$ | 60.49 |
| 1.5043 | 2 | 530 | 61.60 |
| 1.4846 | 5 | 024 | 62.51 |
| 1.4649 | 8 | $\bar{6}24$ | 63.45 |
| | | | |
| 1.4620 | 11 | $\bar{3}15$ | 63.59 |
| 1.4601 | 8 | 332 | 63.68 |
| 1.3854 | 6 | $\bar{3}34,\bar{5}31$ | 67.56 |
| 1.3803 | 5 | $\bar{8}22,\bar{7}11$ | 67.84 |
| 1.3715 | 2 | $\bar{4}41$ | 68.34 |
| | | | |
| 1.3384 | 5 | $\bar{9}12,\bar{7}15$ | 70.27 |
| 1.3337 | 4 | 913 | 70.56 |
| 1.3075 | 4 | $314,\bar{2}43$ | 72.19 |
| 1.3000 | 3 | $\bar{6}25$ | 72.67 |

Sodium bromide chloride, $\text{NaBr}_{.33}\text{Cl}_{.67}$

Sample

The sample was prepared by melting a 1:2 mixture of NaBr and NaCl. After grinding it was annealed for 18 hours at 600 °C in a sealed glass tube.

Color

Colorless

Optical data

Isotropic, N=1.577

Structure

Cubic, Fm3m (225), Z=4. There is a complete solid solution between NaBr and NaCl [Gromakov and Gromakova, 1955].

NBS lattice constant:

$$a = 5.7614(2)\text{\AA}$$

Density

(calculated) 2.54 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 4.2$$

| Internal standard W, $a = 3.16516 \text{\AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|--|-----|-------|-----------------|
| $d (\text{\AA})$ | I | hkl | $2\cdot(\circ)$ |
| 3.329 | 30 | 111 | 26.76 |
| 2.882 | 100 | 200 | 31.00 |
| 2.037 | 45 | 220 | 44.43 |
| 1.7373 | 6 | 311 | 52.64 |
| 1.6632 | 11 | 222 | 55.18 |
| 1.4401 | 5 | 400 | 64.67 |
| 1.3216 | 2 | 331 | 71.30 |
| 1.2883 | 9 | 420 | 73.44 |
| 1.1761 | 5 | 422 | 81.83 |
| 1.1089 | 1 | 511 | 88.00 |
| 1.0185 | 1 | 440 | 98.28 |
| 0.9739 | <1 | 531 | 104.54 |
| .9603 | 1 | 600 | 106.67 |
| .9108 | 1 | 620 | 115.49 |
| .8686 | 1 | 622 | 124.95 |
| .8317 | <1 | 444 | 135.68 |
| .8067 | <1 | 711 | 145.43 |
| .7990 | <1 | 640 | 149.18 |

Reference

Gromakov, S.P. and Gromakova, L.M. (1955). Zh.Fiz. Khim. 29, 746.

Sodium bromide chloride, $\text{NaBr}_{.67}\text{Cl}_{.33}$

Sample

The sample was prepared by melting a 2:1 mixture of NaBr and NaCl. After grinding it was annealed for 18 hours at 600 °C in a sealed glass tube.

Color

Colorless

Optical data

Isotropic, $N = 1.610$

Structure

Cubic, $\text{Fm}3\text{m}$ (225), $Z=4$. There is a complete solid solution series between NaBr and NaCl [Gromakov and Gromakova, 1955].

NBS lattice constant:
 $a = 5.8676(2)\text{\AA}$

Density

(calculated) 2.87 g/cm^3

Reference intensity

$I/I_{\text{corundum}} = 5.5$

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ \text{ C}$ | | | |
|--|-----|-------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\gamma (\text{°})$ |
| 3.387 | 60 | 111 | 26.29 |
| 2.933 | 100 | 200 | 30.45 |
| 2.0742 | 60 | 220 | 43.60 |
| 1.7692 | 12 | 311 | 51.62 |
| 1.6944 | 18 | 222 | 54.08 |
| 1.4669 | 6 | 400 | 63.35 |
| 1.3463 | 4 | 331 | 69.80 |
| 1.3121 | 15 | 420 | 71.90 |
| 1.1977 | 9 | 422 | 80.05 |
| 1.1292 | 3 | 511 | 86.02 |
| 1.0375 | 2 | 440 | 95.88 |
| .9918 | 2 | 531 | 101.91 |
| .9780 | 4 | 600 | 103.93 |
| .9277 | 3 | 620 | 112.26 |
| .8949 | <1 | 533 | 118.80 |
| .8846 | 2 | 622 | 121.09 |
| .8216 | <1 | 711 | 139.28 |
| .8136 | 1 | 640 | 142.42 |

References

Gromakov, S. P. and Gromakova, L. M. (1955). Zh. Fiz. Khim. 29, 746.

Sodium carbonate sulfate, $\text{Na}_4\text{CO}_3\text{SO}_4$

Sample

The sample was prepared by melting together equal molar amounts of Na_2CO_3 and Na_2SO_4 .

Major impurities

~ .05% Ag, Al, Ca, K and Si.

Color

Colorless

Optical data

Uniaxial (-), $N \approx 1.45$

Structure

Hexagonal, $P\bar{3}ml$ (164), $Z=1$, isostructural with Na_2SO_4 , form I, and with $\alpha\text{-Na}_2\text{CO}_3$. A continuous isomorphous series exists in all proportions from zero to 75 mol. percent Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

$$a = 5.2284(5) \text{ \AA}$$

$$c = 6.8808(8)$$

Density
(calculated) 2.528 g/cm^3

Reference intensity
 $I/I_{\text{corundum}} = 1.1$

Polymorphism

The 1:1 composition may occur in several other crystal forms [Klapova and Kovaleva, 1963].

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
|---|-----|-------|--------------------------|
| $d (\text{\AA})$ | I | hkl | $2\cdot (\text{)}^\circ$ |
| 4.528 | 7 | 100 | 19.59 |
| 3.783 | 60 | 101 | 23.50 |
| 3.440 | 45 | 002 | 25.88 |
| 2.741 | 100 | 102 | 32.64 |
| 2.614 | 70 | 110 | 34.28 |
| 2.263 | 2 | 200 | 39.80 |
| 2.150 | 14 | 201 | 41.98 |
| 1.891 | 35 | 202 | 48.07 |
| 1.720 | 8 | 004 | 53.20 |
| 1.710 | 4 | 210 | 53.53 |
| 1.611 | 1 | 203 | 57.14 |
| 1.5322 | 9 | 212 | 60.36 |
| 1.5094 | 6 | 300 | 61.37 |
| 1.4366 | 8 | 114 | 64.85 |
| 1.3825 | 1 | 302 | 67.72 |
| 1.3722 | 1 | 213 | 68.30 |
| 1.3166 | 1 | 105 | 71.61 |
| 1.3073 | 6 | 220 | 72.20 |
| 1.2218 | 5 | 222 | 78.17 |
| 1.1796 | 3 | 312 | 81.54 |
| 1.1467 | 1 | 006 | 84.40 |
| 1.1347 | 3 | 304 | 85.51 |
| 1.1119 | 1 | 106 | 87.70 |
| 1.1016 | 1 | 313 | 88.73 |
| 1.0753 | 2 | 402 | 91.51 |
| 1.0407 | 2 | 224 | 95.49 |

References

- Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.
- Klapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
- Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. 58, 846.

Sodium carbonate sulfate (burkeite), $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$

Sample

The sample was precipitated by mixing boiling aqueous solutions of Na_2CO_3 and Na_2SO_4 in a molar ratio of 1:2. Chemical analysis of the precipitate indicated a ratio of 1:2.0.

Color

Colorless

Structure

Orthorhombic, $Z=4/3$. Ramsdell [1942] reported a cell with the a and b parameters tripled. No evidence was seen here for an enlarged cell. This phase occurs over a range of solid solution [Caspari, 1924] [Schroeder et al., 1936]. Klapova and Burovaya [1957] reported that this phase ("rhombic" burkeite) contained essential H_2O . However the weight loss found at NBS between 350 and 700 °C was only 0.32% after the material had been transformed to the hexagonal form of the α - Na_2SO_4 type.

NBS lattice constants:

$$\begin{aligned}a &= 7.055(2)\text{\AA} \\b &= 9.215(2) \\c &= 5.167(1)\end{aligned}$$

Density

(calculated) 2.571 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 0.7$$

Polymorphism

In studies of the system Na_2CO_3 - Na_2SO_4 Klapova and Burovaya [1957] and Klapova and Kovaleva [1963] found three hexagonal polymorphs of the 1:2 composition, not including this one which they considered a hydrate. Transitions were reported to occur at 400 and 575 °C.

Additional patterns

1. PDF card 2-840 [Michigan Alkali Co. Wyandotte Michigan].
2. Ramsdell [1939].

References

- Caspari, W. A. (1924). J. Chem. Soc. 125, 2381.
 Klapova, A.N. and Burovaya, E.E. (1957). Russ. J. Inorg. Chem. (English Transl.) 2, No.8, 249.
 Klapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
 Ramsdell, L.S. (1939). Am. Mineralogist 24, 109.
 Ramsdell, L.S. (1942). Am. Mineralogist 27, 230.

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25 °C | | | |
|---|-----|-----------|----------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{°})$ |
| 9.215 | 8 | 010 | 9.59 |
| 4.607 | 5 | 020 | 19.25 |
| 4.507 | 17 | 011 | 19.68 |
| 4.172 | 4 | 101 | 21.28 |
| 3.854 | 40 | 120 | 23.06 |
| 3.795 | 75 | 111 | 23.42 |
| 3.526 | 80 | 200 | 25.24 |
| 3.439 | 19 | 021 | 25.89 |
| 3.307 | 3 | 210 | 26.99 |
| 3.072 | 17 | 030 | 29.04 |
| 2.801 | 100 | 220 | 31.93 |
| 2.777 | 55 | 211 | 32.21 |
| 2.640 | 75 | 031 | 33.93 |
| 2.583 | 75 | 002 | 34.70 |
| 2.488 | 5 | 012 | 36.07 |
| 2.345 | 6 | 112 | 38.35 |
| 2.305 | 11 | 040 | 39.05 |
| 2.279 | 4 | 310 | 39.51 |
| 2.191 | 3 | 140 | 41.17 |
| 2.147 | 14 | 122 | 42.04 |
| 2.142 | 11 | 301 | 42.15 |
| 2.105 | 6 | 041 | 42.94 |
| 1.978 | 12 | 032 | 45.84 |
| 1.929 | 30 | 240 | 47.07 |
| 1.904 | 25 | 132 | 47.74 |
| 1.898 | 30 | 222 | 47.88 |
| 1.784 | 2 | 150 | 51.17 |
| 1.764 | 17 | 400 | 51.79 |
| 1.735 | 8 | 051 | 52.71 |
| 1.722 | 3 | 003 | 53.15 |
| 1.673 | 2 | 103 | 54.83 |
| 1.645 | 3 | 113, 340+ | 55.85 |
| 1.635 | 4 | 250 | 56.20 |
| 1.627 | 4 | 322 | 56.53 |
| 1.614 | 4 | 023 | 57.00 |
| 1.557 | 5 | 251 | 59.30 |
| 1.548 | 6 | 203 | 59.67 |
| 1.545 | 5 | 242 | 59.82 |
| 1.536 | 6 | 060 | 60.20 |
| 1.526 | 5 | 213 | 60.64 |
| 1.503 | 6 | 033 | 61.67 |

Sodium carbonate sulfate, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$

Sample

The sample was prepared by melting a 1:2 molar mixture of Na_2CO_3 and Na_2SO_4 . The sample was somewhat hygroscopic.

Color

Colorless

Structure

Hexagonal, $P\bar{3}ml$ (164), $Z = \frac{2}{3}$, isostructural with Na_2SO_4 , form I, and with $\alpha\text{-Na}_2\text{CO}_3$. A continuous series of isomorphous phases occurs in all proportions from zero to 75 mol. percent of Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:

$$a = 5.2624(4) \text{\AA}$$

$$c = 7.0236(7)$$

Density

(calculated) 2.563 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} = 1.1$$

Polymorphism

This composition may occur in several other crystal forms [Khlapova and Kovaleva, 1963].

References

- Gossner, B. (1928). Neues Jahrb. Mineral. Geol., Beilage Bd. 57A, 89.
- Khlapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
- Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. 58, 846.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ\text{C}$ | | | |
|--|-----|-------|------------------|
| $d (\text{\AA})$ | I | hkl | $2\cdot (\circ)$ |
| 4.558 | 10 | 100 | 19.46 |
| 3.824 | 85 | 101 | 23.24 |
| 3.515 | 50 | 002 | 25.32 |
| 2.783 | 100 | 102 | 32.14 |
| 2.631 | 80 | 110 | 34.05 |
| 2.279 | 4 | 200 | 39.51 |
| 2.167 | 11 | 201 | 41.65 |
| 2.106 | 1 | 112 | 42.90 |
| 1.912 | 40 | 202 | 47.51 |
| 1.755 | 10 | 004 | 52.06 |
| 1.7227 | 3 | 210 | 53.12 |
| 1.6332 | 2 | 203 | 56.28 |
| 1.5471 | 11 | 212 | 59.72 |
| 1.5190 | 7 | 300 | 60.94 |
| 1.4848 | 1 | 301 | 62.50 |
| 1.4603 | 10 | 114 | 63.67 |
| 1.3949 | 2 | 302 | 67.04 |
| 1.3876 | 2 | 213 | 67.44 |
| 1.3424 | 1 | 105 | 70.03 |
| 1.3154 | 5 | 220 | 71.69 |
| 1.2639 | 1 | 310 | 75.10 |
| 1.2439 | 1 | 311 | 76.52 |
| 1.2318 | 2 | 222 | 77.41 |
| 1.1892 | 3 | 312 | 80.74 |
| 1.1706 | 1 | 006 | 82.30 |
| 1.1488 | 4 | 304 | 84.21 |
| 1.1337 | 2 | 106 | 85.60 |
| 1.1121 | 2 | 313 | 87.68 |
| 1.0887 | <1 | 215 | 90.07 |
| 1.0837 | 2 | 402 | 90.60 |
| 1.0529 | 2 | 224 | 94.04 |
| 1.0409 | <1 | 206 | 95.47 |

Sodium carbonate sulfate, $\text{Na}_6(\text{CO}_3)_2\text{SO}_4$

Sample

The sample was prepared by melting Na_2CO_3 and Na_2SO_4 together in a 2:1 molar ratio.

Major impurities

~ .05% Ca

Color

Colorless

Structure

Hexagonal, $P\bar{3}ml$ (164), $Z = \frac{2}{3}$, isostructural with Na_2SO_4 , form I, and with $\alpha\text{-Na}_2\text{CO}_3$. A continuous isomorphous series exists in all proportions from zero to 75 mol. percent Na_2CO_3 [Schroeder et al., 1936]. The structure of this type of compound was determined by Gossner [1928].

NBS lattice constants:
 $a = 5.2034(5)\text{\AA}$
 $c = 6.683(1)$

Density
 (calculated) 2.501 g/cm^3

Reference intensity
 $I/I_{\text{corundum}} = 0.7$

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ \text{ C}$ | | | |
|--|-----|-------|---------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 4.505 | 4 | 100 | 19.69 |
| 3.739 | 45 | 101 | 23.78 |
| 3.341 | 55 | 002 | 26.66 |
| 2.684 | 100 | 102 | 33.35 |
| 2.603 | 75 | 110 | 34.43 |
| 2.253 | 2 | 200 | 39.99 |
| 2.135 | 25 | 201 | 42.29 |
| 1.868 | 35 | 202 | 48.72 |
| 1.7034 | 5 | 210 | 53.77 |
| 1.6707 | 6 | 004 | 54.91 |
| 1.6508 | 2 | 211 | 55.63 |
| 1.5836 | 2 | 203 | 58.21 |
| 1.5181 | 6 | 212 | 60.98 |
| 1.5019 | 6 | 300 | 61.71 |
| 1.4655 | 1 | 301 | 63.42 |
| 1.4062 | 4 | 114 | 66.43 |
| 1.3527 | 1 | 213 | 69.42 |
| 1.3008 | 5 | 220 | 72.62 |
| 1.2814 | <1 | 105 | 73.90 |
| 1.2453 | 1 | 303 | 76.42 |
| 1.2125 | 3 | 222 | 78.88 |
| 1.1706 | 3 | 312 | 82.30 |

Polymorphism

This composition may occur in several other crystal forms [Klapova and Kovaleva, 1963].

References

- Gossner, B. (1928). Neues Jahrb. Mineral., Beilage Bd. 57A, 89.
- Klapova, A. N. and Kovaleva, E. S. (1963). J. Struct. Chem. USSR (Eng. Transl.) 4, 517.
- Schroeder, W.C., Berk, A.A., Partridge, E.P., and Gabriel, A. (1936). J. Am. Chem. Soc. 58, 846.

Sodium chromium oxide sulfate, $\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$

Sample

The sample was prepared by melting an equimolar mixture of Na_2SO_4 and Na_2CrO_4 . This material was then annealed for 18 hours at 600 °C, followed by 350 °C for 2 hours in a stream of oxygen.

Color

Brilliant greenish yellow

Structure

Orthorhombic, Amam (63), $Z=2$, isostructural with Na_2CrO_4 and Na_2SO_4 (III) [Fischmeister, 1954]. The structure of Na_2CrO_4 was determined by Miller [1936], and the space group was corrected by Niggli [1954]. Na_2CrO_4 and Na_2SO_4 (III) form a complete isomorphous series [Fischmeister, 1954].

NBS lattice constants:

$$\begin{aligned} a &= 7.055(2)\text{\AA} \\ b &= 9.115(2) \\ c &= 5.744(2) \end{aligned}$$

Density
(calculated) 2.733 g/cm³

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

Major impurities
~ .05% Ag and Al

References

- Fischmeister, H. (1954). Acta Cryst. 7, 776.
- Miller, J.J. (1936). Z. Krist. 94, 131.
- Niggli, A. (1954). Acta Cryst. 7, 776.

| Internal standard Ag, $a = 4.08641 \text{\AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|--|-----|-------|---------------------|
| $d (\text{\AA})$ | I | hkl | $2\cdot (\text{°})$ |
| 4.857 | 15 | 011 | 18.25 |
| 4.555 | 3 | 020 | 19.47 |
| 4.003 | 50 | 111 | 22.19 |
| 3.831 | 45 | 120 | 23.20 |
| 3.527 | 55 | 200 | 25.23 |
| 2.869 | 75 | 002 | 31.15 |
| 2.855 | 100 | 211 | 31.30 |
| 2.687 | 60 | 031 | 33.32 |
| 2.511 | 2 | 131 | 35.73 |
| 2.430 | 20 | 022 | 36.96 |
| 2.280 | 3 | 040 | 39.49 |
| 2.168 | 2 | 140 | 41.62 |
| 2.135 | 6 | 231 | 42.29 |
| 2.116 | 3 | 311 | 42.70 |
| 2.089 | 7 | 320 | 43.28 |
| 2.000 | 16 | 222 | 45.30 |
| 1.915 | 9 | 240 | 47.44 |
| 1.811 | 2 | 113 | 50.34 |
| 1.770 | 10 | 331 | 51.60 |
| 1.764 | 20 | 400 | 51.79 |
| 1.686 | 1 | 151 | 54.31 |
| 1.656 | 4 | 213 | 55.45 |
| 1.619 | 8 | 033 | 56.81 |
| 1.5926 | 10 | 242 | 57.85 |
| 1.5585 | 2 | 251 | 59.24 |
| 1.5032 | 2 | 402 | 61.65 |
| 1.4742 | 10 | 431 | 63.00 |

Sodium magnesium carbonate (eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$

Sample

The sample was made by reacting a saturated solution of sodium hydrogen carbonate with a suspension of basic magnesium carbonate.

Color

Colorless

Optical data

Uniaxial (-), $N_e = 1.450$, $N_o = 1.605$ [Pabst, 1973].

Structure

Hexagonal, $R\bar{3}$ (148), $Z = 3$ [Pabst, 1973]. Eitel and Skaliks [1929] previously reported $P\bar{3}$ (147) as the space group.

NBS lattice constants:

$$a = 4.9423(2)\text{\AA}$$

$$c = 16.396(1)$$

Density

(calculated) 2.792 g/cm^3

Reference intensity

$$\frac{I}{I_{\text{corundum}}} 1.8$$

Additional patterns

1. PDF card 4-737 [Wyandotte Chem. Co., Wyandotte, Michigan]

References

Eitel, W. and Skaliks, W. (1929). Z. anorg. u. allgem. Chem. 183, 263.

Pabst, A. (1973). Am. Mineralogist 58, 211.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
|---|-----|-------------|--------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (^\circ)$ |
| 5.48 | <1 | 003 | 16.17 |
| 3.794 | 16 | 012 | 23.43 |
| 2.731 | 25 | 006 | 32.77 |
| 2.602 | 100 | 015 | 34.44 |
| 2.469 | 25 | 110 | 36.36 |
| 2.251 | 20 | 113 | 40.03 |
| 2.121 | 2 | 021 | 42.58 |
| 2.0710 | 18 | 202 | 43.67 |
| 1.8975 | 20 | 024 | 47.90 |
| 1.8486 | 2 | 018 | 49.25 |
| 1.8333 | 9 | 116 | 49.69 |
| 1.7925 | 9 | 205 | 50.90 |
| 1.6099 | 8 | 211 | 57.17 |
| 1.5873 | 2 | 122 | 58.06 |
| 1.5311 | 11 | 1·0·10 | 60.41 |
| 1.5048 | 1 | 214 | 61.58 |
| 1.4803 | 1 | 208 | 62.71 |
| 1.4663 | 4 | 119 | 63.38 |
| 1.4505 | 6 | 125 | 64.15 |
| 1.4264 | 5 | 300 | 65.37 |
| 1.3802 | <1 | 303 | 67.85 |
| 1.3665 | 1 | 0·0·12 | 68.62 |
| 1.3310 | 1 | 217 | 70.72 |
| 1.3016 | <1 | 0·2·10 | 72.57 |
| 1.2695 | 1 | 128 | 74.71 |
| 1.2355 | 4 | 220 | 77.14 |
| 1.2232 | <1 | 2·0·11 | 78.06 |
| 1.1957 | <1 | 1·1·12 | 80.21 |
| 1.1841 | 1 | 131 | 81.16 |
| 1.1749 | <1 | 312 | 81.93 |
| 1.1516 | 3 | 2·1·10 | 83.96 |
| 1.1297 | <1 | 0·1·14 | 85.98 |
| 1.1233 | <1 | 309 | 86.59 |
| 1.1163 | 4 | 315 | 87.27 |
| 1.0962 | <1 | 1·2·11 | 89.29 |
| 1.0930 | 1 | 0·0·15 | 89.62 |
| 1.0865 | <1 | 0·2·13 | 90.30 |
| 1.0588 | <1 | 137 | 93.35 |
| 1.0353 | <1 | 404 | 96.15 |
| 1.0271 | <1 | 2·0·14, 318 | 97.18 |
| 1.0227 | <1 | 229 | 97.74 |
| 1.0172 | 1 | 045 | 98.44 |
| 0.9996 | <1 | 1·1·15 | 100.82 |
| .9947 | <1 | 2·1·13 | 101.50 |
| .9750 | <1 | 232 | 104.38 |
| .9615 | 1 | 1·3·10 | 106.47 |
| .9550 | <1 | 324 | 107.53 |
| .9488 | <1 | 1·2·14, 048 | 108.55 |
| .9406 | 1 | 235 | 109.95 |
| .9340 | 1 | 410 | 111.12 |

Sodium sulfate, Na_2SO_4

Sample

The sample was prepared by heating Na_2SO_4 at 700 °C for one hour. The sample changes to Na_2SO_4 , form V, if exposed to moist air.

Color

Colorless

Structure

Orthorhombic, Amam (63), $Z=4$, isostructural with Na_2CrO_4 [Frevel, 1940]. The structure of Na_2CrO_4 was determined by Miller [1936]. The space group was corrected by Niggli [1954].

NBS lattice constants:

$$\begin{aligned} a &= 6.9666(9) \text{\AA} \\ b &= 8.9511(9) \\ c &= 5.6109(6) \end{aligned}$$

Density

(calculated) 2.696 g/cm³

Reference intensity

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

Polymorphism

The polymorphism of Na_2SO_4 is complex and not completely resolved. The form reported here is stable at room temperature and has been referred to as Na_2SO_4 , form III; Na_2SO_4 , form I, is hexagonal and is stable above 250°C. [Kracek and Ksanda, 1930]. Klapova [1956] reported a form (δ), stable between 600°C. and the melting point (900°C.). Klapova and Burovaya [1957] discussed the phase of Na_2SO_4 known as form V and as the mineral thenardite. They considered it to be a hydrate.

Additional patterns

1. PDF card 8-31 [Fischmeister, 1954]
2. Das Gupta [1954]

References

- Das Gupta, D. R. (1954). Acta Cryst. 7, 275.
 Fischmeister, H. (1954). Acta Cryst. 7, 776.
 Frevel, L.K. (1940). J. Chem. Phys. 8, 290.
 Klapova, A.N. (1956). Russ. J. Inorg. Chem. (English Transl.) 1, No. 11, 132.
 Klapova, A.N. and Burovaya, E.E. (1957). Russ. J. Inorg. Chem. (English Transl.) 2, No. 8, 249.
 Kracek, F. C. and Ksanda, C. J. (1930). J. Phys. Chem. 34, 1741.
 Miller, J.J. (1936). Z. Krist. 94, 131.
 Niggli, A. (1954). Acta Cryst. 7, 776.

| Internal standard Ag, $a = 4.08641 \text{\AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|--|-----|---------|---------------------|
| $d (\text{\AA})$ | I | hkl | $2\cdot (\text{°})$ |
| 4.759 | 9 | 011 | 18.63 |
| 4.476 | 4 | 020 | 19.82 |
| 3.929 | 35 | 111 | 22.61 |
| 3.768 | 30 | 120 | 23.59 |
| 3.485 | 25 | 200 | 25.54 |
| 2.809 | 100 | 211,002 | 31.83 |
| 2.636 | 45 | 031 | 33.98 |
| 2.465 | 2 | 131 | 36.42 |
| 2.377 | 20 | 022 | 37.82 |
| 2.238 | 4 | 040 | 40.26 |
| 2.184 | 2 | 202 | 41.31 |
| 2.131 | 6 | 140 | 42.39 |
| 2.101 | 6 | 231 | 43.01 |
| 2.086 | 7 | 311 | 43.33 |
| 2.062 | 5 | 320 | 43.87 |
| 1.963 | 18 | 222 | 46.20 |
| 1.883 | 9 | 240 | 48.29 |
| 1.831 | 1 | 013 | 49.76 |
| 1.771 | 1 | 113 | 51.56 |
| 1.7496 | 13 | 042 | 52.24 |
| 1.7419 | 18 | 331,400 | 52.49 |
| 1.6964 | 2 | 142 | 54.01 |
| 1.6229 | 3 | 420 | 56.67 |
| 1.6206 | 4 | 213 | 56.76 |
| 1.6115 | 3 | 340 | 57.11 |
| 1.5845 | 9 | 033 | 58.17 |
| 1.5633 | 10 | 242 | 59.04 |
| 1.5320 | 3 | 251 | 60.37 |
| 1.4919 | 1 | 060 | 62.17 |
| 1.4799 | 2 | 402 | 62.73 |
| 1.4528 | 9 | 431 | 64.04 |
| 1.4425 | 2 | 233 | 64.55 |
| 1.4028 | 4 | 004 | 66.61 |
| 1.3748 | 3 | 351,440 | 68.15 |
| 1.3370 | 1 | 511 | 70.36 |
| 1.3302 | 2 | 520 | 70.77 |
| 1.3168 | 3 | 062 | 71.60 |
| 1.3144 | 2 | 124 | 71.75 |
| 1.2941 | 3 | 162 | 73.06 |
| 1.2714 | 2 | 153 | 74.58 |
| 1.2494 | 1 | 224 | 76.12 |
| 1.2317 | 2 | 262,531 | 77.42 |

Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$

Sample

The sample was prepared by heating $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ at 60 - 70 °C for several hours under vacuum.

Color
Colorless

Structure

Monoclinic, Cc (9) or C2/c (15), Z=4. The structure was determined by Jensen [1942].

NBS lattice constant:

$$\begin{aligned}a &= 11.688(1)\text{\AA} \\b &= 6.4048(5) \\c &= 6.6957(6) \\&\beta = 105.54(1)^\circ\end{aligned}$$

Density
(calculated) 2.676 g/cm³

Reference intensity
 $I/I_{\text{corundum}} = 1.0$

Additional patterns

1. PDF card 3-500 [Jensen, 1942].

References

Jensen, A.T.(1942). Kgl. Danske Videnskab. Selskab
Mat. Fys. Medd. 20, Nr.5.

| Internal standard W, a = 3.16516 Å CuK α_1 , $\lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
|---|-----|---------|--------|
| d (Å) | I | hkl | 2· (°) |
| 5.63 | 60 | 200 | 15.74 |
| 4.523 | 75 | 111 | 19.61 |
| 3.964 | 35 | 111 | 22.41 |
| 3.238 | 35 | 310 | 27.52 |
| 3.229 | 30 | 002 | 27.60 |
| 3.206 | 100 | 311,020 | 27.80 |
| 2.966 | 4 | 112 | 30.10 |
| 2.871 | 20 | 021 | 31.13 |
| 2.816 | 2 | 400 | 31.75 |
| 2.784 | 45 | 220 | 32.12 |
| 2.690 | 30 | 221 | 33.28 |
| 2.659 | 75 | 311 | 33.68 |
| 2.645 | 40 | 112 | 33.86 |
| 2.608 | 20 | 312 | 34.36 |
| 2.523 | 35 | 202 | 35.55 |
| 2.475 | 30 | 402 | 36.27 |
| 2.442 | 14 | 221 | 36.78 |
| 2.272 | 30 | 022 | 39.63 |
| 2.261 | 35 | 222 | 39.84 |
| 2.189 | 13 | 511 | 41.20 |
| 2.140 | 1 | 421 | 42.19 |
| 2.125 | 2 | 510 | 42.51 |
| 2.114 | 35 | 420 | 42.74 |
| 2.101 | 40 | 113 | 43.01 |
| 2.025 | 30 | 512,131 | 44.71 |
| 2.020 | 30 | 313 | 44.83 |
| 1.982 | 9 | 222 | 45.74 |
| 1.966 | 30 | 131 | 46.13 |
| 1.959 | 5 | 422 | 46.31 |
| 1.922 | 6 | 113 | 47.25 |
| 1.900 | 2 | 421 | 47.84 |
| 1.8816 | 20 | 511 | 48.33 |
| 1.8765 | 18 | 600 | 48.47 |
| 1.8522 | 13 | 602 | 49.15 |
| 1.7481 | 2 | 513 | 52.29 |
| 1.7236 | 2 | 331 | 53.09 |
| 1.7096 | 1 | 332 | 53.56 |
| 1.6866 | 2 | 423 | 54.35 |
| 1.6640 | 7 | 621 | 55.15 |
| 1.6253 | 8 | 422 | 56.58 |
| 1.6190 | 7 | 620 | 56.82 |
| 1.6151 | 6 | 111 | 56.97 |
| 1.6066 | 6 | 114 | 57.30 |
| 1.6020 | 6 | 223,040 | 57.48 |
| 1.5979 | 10 | 314,512 | 57.64 |
| 1.5740 | 6 | 712,531 | 58.60 |
| 1.5599 | 3 | 710 | 59.18 |
| 1.5401 | 8 | 133,240 | 60.02 |
| 1.5240 | 7 | 332,241 | 60.72 |
| 1.5072 | 4 | 533 | 61.47 |

Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$ – continued

| d (\AA) | I | hkl | $2\cdot (\circ)$ |
|----------------------|-----|----------|------------------|
| 1.4833 | 6 | 224 | 62.57 |
| 1.4765 | 4 | 514 | 62.89 |
| 1.4651 | 8 | 133 | 63.44 |
| 1.4609 | 6 | 602 | 63.64 |
| 1.4554 | 4 | 713 | 63.91 |
| 1.4507 | 6 | 204 | 64.14 |
| 1.4401 | 5 | 024 | 64.67 |
| 1.4342 | 6 | 042, 711 | 64.97 |
| 1.4309 | 10 | 242 | 65.14 |
| 1.4270 | 5 | 604 | 65.34 |
| 1.4073 | 5 | 800 | 66.37 |
| 1.3916 | 7 | 440 | 67.22 |
| 1.3836 | 9 | 533 | 67.66 |
| 1.3502 | 8 | 513 | 69.57 |
| 1.3443 | 4 | 442 | 69.92 |
| 1.3289 | 8 | 622 | 70.85 |
| 1.3252 | 5 | 441 | 71.08 |
| 1.3208 | 9 | 333 | 71.35 |
| 1.3149 | 5 | 731 | 71.72 |
| 1.3127 | 3 | 822 | 71.86 |
| 1.3034 | 6 | 714, 624 | 72.45 |
| 1.2948 | 3 | 115 | 73.01 |
| 1.2886 | 3 | 820 | 73.42 |
| 1.2726 | 4 | 150 | 74.50 |
| 1.2691 | 5 | 911 | 74.74 |
| 1.2558 | 4 | 151 | 75.67 |
| 1.2523 | 5 | 515 | 75.92 |
| 1.2488 | 5 | 134, 823 | 76.17 |
| 1.2416 | 3 | 151 | 76.69 |
| 1.2280 | 2 | 910 | 77.70 |
| 1.2244 | 2 | 733 | 77.97 |
| 1.2208 | 6 | 442 | 78.24 |
| 1.2112 | 8 | 731, 642 | 78.98 |

Strontium chloride hydroxide phosphate, $\text{Sr}_5\text{Cl}_{1.65}(\text{OH})_{.35}(\text{PO}_4)_3$

Sample

The sample was prepared by adding a Na_3PO_4 solution to a saturated solution of SrCl_2 . After boiling, the precipitate was filtered, washed, dried, and heated to 1100 °C for one half hour. Analysis showed 3.07 percent chlorine.

Color

Colorless

Structure

Hexagonal, $P6_3/m$ (176), $Z=2$, isostructural with calcium hydroxyapatite, $\text{Ca}_5\text{OH}(\text{PO}_4)_3$; its structure was determined by Posner et al. [1958]. There is a complete solid solution between $\text{Sr}_5\text{OH}(\text{PO}_4)_3$ and $\text{Sr}_5\text{Cl}(\text{PO}_4)_3$. However, the structure of $\text{Ca}_5\text{Cl}(\text{PO}_4)_3$ was determined by Mackie et al. [1972] and found to be monoclinic, pseudo-hexagonal. The data here gave no indication of a departure from hexagonal.

NBS lattice constants:

$$\begin{aligned}a &= 9.847(1)\text{\AA} \\c &= 7.219(1)\end{aligned}$$

Density

(calculated) 4.119 g/cm³

Reference intensity

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

Additional patterns

- PDF 16-666 [General Electric Co. Ltd., Wembley England - for $\text{Sr}_5\text{Cl}(\text{PO}_4)_3$].

References

- Mackie, P.E., Elliott, J.C., and Young, R.A. (1972)
Acta Cryst. B28, 1840.
Posner, A.S., Perloff, A., and Diorio, A.F. (1958)
Acta Cryst. 11, 308.

| Internal standard W, $a = 3.16516 \text{\AA}$ | | | |
|---|-----|-------|--------------------|
| $\text{CuK}\alpha_1 \lambda = 1.54056 \text{\AA}$; temp. 25 °C | | | |
| $d (\text{\AA})$ | I | hkl | $2\cdot(\text{°})$ |
| 8.51 | 2 | 100 | 10.39 |
| 5.50 | 2 | 101 | 16.10 |
| 4.93 | 3 | 110 | 17.98 |
| 4.263 | 13 | 200 | 20.82 |
| 4.070 | 9 | 111 | 21.82 |
| 3.609 | 13 | 002 | 24.65 |
| 3.325 | 11 | 102 | 26.79 |
| 3.225 | 20 | 210 | 27.64 |
| 2.942 | 95 | 211 | 30.36 |
| 2.910 | 100 | 112 | 30.70 |
| 2.842 | 55 | 300 | 31.45 |
| 2.755 | 3 | 202 | 32.47 |

| $d (\text{\AA})$ | I | hkl | $2\cdot(\text{°})$ |
|------------------|-----|----------|--------------------|
| 2.645 | 1 | 301 | 33.86 |
| 2.464 | 1 | 220 | 36.44 |
| 2.404 | 2 | 212 | 37.37 |
| 2.365 | 9 | 310 | 38.02 |
| 2.247 | 2 | 311 | 40.10 |
| 2.232 | 6 | 302 | 40.37 |
| 2.162 | 9 | 113 | 41.75 |
| 2.132 | 2 | 400 | 42.35 |
| 2.096 | 2 | 203 | 43.12 |
| 2.033 | 35 | 222 | 44.52 |
| 1.978 | 11 | 312 | 45.83 |
| 1.956 | 4 | 329 | 46.39 |
| 1.928 | 25 | 213 | 47.10 |
| 1.888 | 15 | 321 | 48.16 |
| 1.861 | 15 | 410 | 48.90 |
| 1.835 | 14 | 402, 303 | 49.63 |
| 1.804 | 9 | 004 | 50.54 |
| 1.721 | <1 | 223, 322 | 53.18 |
| 1.695 | 1 | 114 | 54.07 |
| 1.687 | 2 | 313 | 54.32 |
| 1.662 | 1 | 204 | 55.22 |
| 1.655 | 4 | 412 | 55.49 |
| 1.640 | 1 | 330 | 56.02 |
| 1.6120 | 3 | 420 | 57.09 |
| 1.6004 | 2 | 331 | 57.54 |
| 1.5745 | 5 | 214 | 58.58 |
| 1.5417 | 3 | 502 | 59.95 |
| 1.5318 | 1 | 510 | 60.38 |
| 1.5236 | 10 | 304 | 60.74 |
| 1.5186 | 10 | 323 | 60.96 |
| 1.4975 | 7 | 511 | 61.91 |
| 1.4943 | 7 | 332 | 62.06 |
| 1.4725 | 1 | 413, 422 | 63.08 |
| 1.4346 | <1 | 314 | 64.95 |
| 1.4101 | 1 | 512 | 66.22 |
| 1.3775 | 2 | 404 | 68.00 |
| 1.3658 | 1 | 520 | 68.66 |
| 1.3563 | 1 | 333 | 69.21 |
| 1.3418 | 2 | 521 | 70.07 |
| 1.3389 | 3 | 423 | 70.24 |
| 1.3261 | 2 | 324 | 71.02 |
| 1.3224 | 3 | 602 | 71.25 |
| 1.3178 | 4 | 215 | 71.54 |
| 1.3067 | 2 | 432 | 72.24 |
| 1.2954 | 9 | 414 | 72.97 |
| 1.2774 | 7 | 522 | 74.17 |
| 1.2310 | 3 | 440 | 77.47 |
| 1.2142 | 1 | 334 | 78.75 |
| 1.2115 | 1 | 433 | 78.96 |
| 1.2021 | 3 | 424 | 79.70 |
| 1.1875 | 1 | 523 | 80.88 |
| 1.1680 | 4 | 514 | 82.52 |
| 1.1618 | 2 | 325 | 83.06 |
| 1.1543 | 2 | 532 | 83.72 |

Strontium oxide hydrate, $\text{SrO}_2 \cdot 8\text{H}_2\text{O}$

Sample

A solution of SrCl_2 was treated with a slight excess of three percent H_2O_2 and stirred. Dilute NH_4OH solution was added and the precipitate was dried at room temperature. Since the crystals were very thin platelets, orientation may have affected intensity measurements.

Color

Colorless

Structure

Tetragonal, $P4/mcc$ (124), $Z=2$. The structure was determined by Vannerberg [1959].

NBS lattice constants:

$$a = 6.3432(5)\text{\AA}$$

$$c = 11.197(1)$$

Density

(calculated) 1.944 g/cm^3

Additional patterns

1. PDF card 12-521 [Vannerberg, 1959].
2. PDF card 2-1245 [Natta, 1932].

References

- Natta, G. (1932). *Gazz. Chim. Ital.* 62, 444.
 Vannerberg, N-G. (1959). *Arkiv Kemi* 14, 17.

| Internal standard W, $a = 3.16516 \text{ \AA}$ $\text{CuK}\alpha_1 \lambda = 1.54056 \text{ \AA}$; temp. 25°C | | | |
|---|-----|-------|-------------------------|
| $d (\text{\AA})$ | I | hkl | $2\psi (\text{)}^\circ$ |
| 6.36 | 2 | 100 | 13.92 |
| 5.59 | 100 | 002 | 15.85 |
| 4.49 | 2 | 110 | 19.74 |
| 4.197 | 7 | 102 | 21.15 |
| 3.496 | 9 | 112 | 25.46 |
| 2.798 | 10 | 004 | 31.96 |
| 2.759 | 4 | 202 | 32.42 |
| 2.750 | 4 | 211 | 32.53 |
| 2.560 | 9 | 104 | 35.02 |
| 2.530 | 2 | 212 | 35.45 |
| 2.377 | 11 | 114 | 37.82 |
| 2.258 | 2 | 213 | 39.89 |
| 2.242 | 1 | 220 | 40.18 |
| 2.098 | 5 | 204 | 43.09 |
| 2.081 | 1 | 222 | 43.45 |
| 2.007 | 2 | 310 | 45.14 |
| 1.992 | 5 | 214 | 45.50 |

| $d (\text{\AA})$ | I | hkl | $2\psi (\text{)}^\circ$ |
|------------------|-----|-------------|-------------------------|
| 1.979 | <1 | 302 | 45.81 |
| 1.889 | 2 | 312 | 48.14 |
| 1.866 | 1 | 006 | 48.75 |
| 1.791 | 8 | 106 | 50.95 |
| 1.758 | 1 | 320, 215 | 51.97 |
| 1.723 | 1 | 116 | 53.10 |
| 1.687 | <1 | 304 | 54.32 |
| 1.678 | <1 | 322 | 54.64 |
| 1.608 | <1 | 206 | 57.23 |
| 1.559 | 4 | 216 | 59.20 |
| 1.526 | <1 | 402 | 60.64 |
| 1.490 | <1 | 324 | 62.24 |
| 1.444 | <1 | 332 | 64.48 |
| 1.434 | <1 | 226 | 64.94 |
| 1.418 | <1 | 420 | 65.81 |
| 1.399 | 4 | 008, 306 | 66.79 |
| 1.394 | 1 | 217 | 67.11 |
| 1.379 | 1 | 404 | 67.90 |
| 1.374 | 1 | 422 | 68.18 |
| 1.367 | 4 | 108, 316 | 68.62 |
| 1.348 | <1 | 414 | 69.67 |
| 1.336 | <1 | 118 | 70.41 |
| 1.319 | <1 | 334 | 71.47 |
| 1.280 | <1 | 208, 326 | 73.98 |
| 1.255 | 1 | 218 | 75.71 |
| 1.187 | 1 | 228, 416 | 80.93 |
| 1.167 | 1 | 308, 336 | 82.59 |
| 1.155 | <1 | 434 | 83.63 |
| 1.153 | <1 | 522 | 83.85 |
| 1.148 | 1 | 318 | 84.30 |
| 1.139 | <1 | 219 | 85.09 |
| 1.120 | <1 | 0·0·10 | 86.91 |
| 1.103 | 1 | 1·0·10 | 88.61 |
| 1.095 | 1 | 328 | 89.41 |
| 1.086 | <1 | 1·1·10 | 90.33 |
| 1.056 | <1 | 2·0·10 | 93.67 |
| 1.0414 | 1 | 2·1·10 | 95.40 |
| 1.0352 | 1 | 418, 516 | 96.16 |
| 1.0014 | <1 | 2·2·10 | 100.56 |
| .9960 | 1 | 428, 526 | 101.31 |
| .9891 | <1 | 604 | 102.30 |
| .9774 | <1 | 3·1·10, 614 | 104.01 |
| .9754 | <1 | 542 | 104.31 |
| .9580 | <1 | 2·1·11 | 107.04 |
| .9446 | <1 | 3·2·10 | 109.27 |
| .9398 | <1 | 438, 536 | 110.10 |
| .9231 | <1 | 1·0·12 | 113.12 |
| .9133 | <1 | 1·1·12 | 115.00 |
| .9053 | <1 | 4·1·10 | 116.60 |
| .9012 | <1 | 528 | 117.44 |
| .8952 | <1 | 2·0·12 | 118.73 |
| .8862 | <1 | 2·1·12 | 120.72 |

Strontium phosphate, alpha Sr₂P₂O₇

Sample

The sample was prepared by adding dilute NH₄OH to a hot concentrated aqueous solution of SrCl₂ and Na₃PO₄. The precipitate was filtered, washed with alcohol, and heated to 1200 °C for ten minutes.

Major impurities

~ .05% Al, Ba, Ca, Mg, Co, and V.

Color

Colorless

Structure

Orthorhombic, Z=4, isostructural with α-Ca₂P₂O₇ [Wanmaker and ter Vrugt, 1967], [Ranby et al. 1955].

NBS lattice constants:

$$\begin{aligned}a &= 8.917(2) \text{ Å} \\b &= 13.169(2) \\c &= 5.400(1)\end{aligned}$$

Density
(calculated) 3.657 g/cm³

Reference intensity

$$I/I_{\text{corundum}} = 2.3$$

Polymorphism

The alpha form is stable above 750 °C [Ranby et al., 1955]. Below 750 °C the alpha form very slowly changes to the beta form. The beta form is represented by PDF card 13-194 [Hoffman and Mooney, 1960].

Additional patterns

1. PDF card 12-362 [Ropp et al., 1959]

| Internal standard Ag, a = 4.08641 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C | | | |
|---|----------|------------|---------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2θ</i> (°) |
| 7.40 | 35 | 110 | 11.95 |
| 6.60 | 13 | 020 | 13.41 |
| 5.30 | 3 | 120 | 16.70 |
| 5.01 | 3 | 011 | 17.70 |
| 4.462 | 11 | 200 | 19.88 |
| 3.940 | 9 | 130 | 22.55 |
| 3.694 | 4 | 220 | 24.07 |
| 3.439 | 85 | 201 | 25.89 |
| 3.406 | 100 | 031 | 26.14 |
| 3.327 | 35 | 211 | 26.77 |
| 3.291 | 4 | 040 | 27.07 |
| 3.182 | 15 | 131 | 28.02 |
| 3.128 | 25 | 230 | 28.51 |
| 3.087 | 2 | 140 | 28.90 |
| 3.048 | 7 | 221 | 29.28 |
| 2.900 | 20 | 310 | 30.81 |
| 2.700 | 45 | 002 | 33.15 |
| 2.680 | 25 | 141 | 33.41 |
| 2.648 | 2 | 240,012 | 33.82 |
| 2.554 | 14 | 311 | 35.11 |
| 2.525 | 11 | 150 | 35.52 |
| 2.422 | 7 | 321 | 37.09 |
| 2.406 | 10 | 122 | 37.35 |
| 2.377 | 2 | 241 | 37.81 |
| 2.310 | 5 | 202 | 38.95 |
| 2.274 | 2 | 212 | 39.60 |
| 2.239 | 6 | 331 | 40.25 |
| 2.230 | 9 | 400 | 40.42 |
| 2.195 | 30 | 060 | 41.08 |
| 2.132 | 6 | 160 | 42.36 |
| 2.090 | 1 | 251 | 43.25 |
| 2.044 | 65 | 232 | 44.27 |
| 1.987 | 7 | 430 | 45.61 |
| 1.982 | 8 | 161 | 45.73 |
| 1.976 | 9 | 312 | 45.88 |
| 1.966 | 11 | 421 | 46.13 |
| 1.913 | 2 | 322 | 47.49 |
| 1.891 | 6 | 242 | 48.08 |
| 1.866 | 17 | 431 | 48.76 |
| 1.850 | 30 | 261 | 49.21 |
| 1.776 | 3 | 071 | 51.40 |
| 1.747 | 4 | 441 | 52.34 |
| 1.742 | 3 | 171 | 52.48 |
| 1.722 | 2 | 520 | 53.15 |
| 1.703 | 8 | 062,450 | 53.79 |
| 1.680 | 6 | 511 | 54.59 |
| 1.669 | 12 | 203 | 54.97 |
| 1.665 | 13 | 033 | 55.10 |
| 1.656 | 4 | 213 | 55.44 |
| 1.651 | 3 | 271 | 55.62 |

Strontium phosphate, alpha $\text{Sr}_2\text{P}_2\text{O}_7$ – continued

| <i>d</i> (\AA) | <i>I</i> | <i>hkl</i> | 2β ($^{\circ}$) |
|---------------------------|----------|------------|-------------------------|
| 1.6402 | 2 | 521 | 56.02 |
| 1.6370 | 3 | 133 | 56.14 |
| 1.6180 | <1 | 223 | 56.86 |
| 1.6009 | 3 | 432 | 57.52 |
| 1.5903 | 7 | 370 | 57.94 |
| 1.5643 | 4 | 460 | 59.00 |
| 1.5554 | 3 | 143 | 59.37 |
| 1.5297 | 3 | 313 | 60.47 |
| 1.5249 | 2 | 371 | 60.68 |
| 1.5026 | 3 | 461 | 61.68 |

References

- Hoffman, C.W.W. and Mooney, R.W. (1960). J. Electro-
chem. Soc. 107, 8541.
Ranby, P.W., Mash, D.H., and Henderson, S.T. (1955).
Brit. J. Appl. Phys. 6, Supplement 4 S18.
Ropp, R.C., Aia, M.A., Hoffman, C.W.W., Veleker,
T.J., and Mooney, R.W. (1959). Anal. Chem. 31,
1163.
Wanmaker, W.L. and ter Vrugt, J.W. (1967). Philips
Res. Rep. 22, 355.

Strontium phosphate, alpha Sr₃(PO₄)₂

Sample

The sample was prepared by heating a 3:2 molar mixture of SrCO₃ and (NH₄)₂HPO₄ at 700°C, grinding, and reheating at 1200 °C for 15 minutes.

Color

Colorless

Structure

Hexagonal, R̄3m (166), Z = 3, isostructural with Ba₃(PO₄)₂. The structure was determined by Zachariasen [1948].

NBS lattice constants:

$$\begin{aligned} a &= 5.3871(2) \text{ Å} \\ c &= 19.780(1) \end{aligned}$$

Density

(calculated) 4.537 g/cm³

Reference intensity

I/I_{corundum} 4.4

Polymorphism

α -Sr₃(PO₄)₂ undergoes a readily reversible, polymorphic inversion at 1305 °C to β -Sr₃(PO₄)₂ [Sarver et al., 1961].

Additional patterns

1. PDF card 14-271 [Sarver et al., 1961].
2. Zachariasen [1948].
3. PDF card 2-744 is for Sr₅OH(PO₄)₃ and not Sr₃(PO₄)₂.

References

Sarver, J. F., Hoffman, M. V., and Hummel, F. A. (1961). J. Electrochem. Soc. 108, 1103.
Zachariasen, W. H. (1948). Acta Cryst. 1, 263.

| Internal standard W, a = 3.16516 Å CuKα ₁ λ = 1.54056 Å; temp. 25 °C | | | |
|--|----------|------------|--------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2</i> (°) |
| 6.60 | 1 | 003 | 13.40 |
| 4.554 | 7 | 101 | 19.52 |
| 4.225 | 1 | 012 | 21.01 |
| 3.393 | 10 | 104 | 26.24 |
| 3.016 | 100 | 015 | 29.59 |
| 2.694 | 85 | 110 | 33.23 |
| 2.494 | <1 | 113 | 35.98 |
| 2.418 | <1 | 107 | 37.15 |
| 2.318 | 3 | 021 | 38.82 |
| 2.271 | 11 | 202 | 39.66 |
| 2.198 | 11 | 009 | 41.03 |
| 2.186 | 2 | 018 | 41.27 |
| 2.110 | 14 | 024 | 42.82 |
| 2.087 | 7 | 116 | 43.32 |
| 2.009 | 35 | 205 | 45.08 |
| 1.821 | 20 | 1·0·10 | 50.05 |
| 1.799 | 2 | 027 | 50.69 |
| 1.7565 | 2 | 211 | 52.02 |
| 1.7360 | <1 | 122 | 52.68 |
| 1.7031 | 9 | 119 | 53.78 |
| 1.6607 | 1 | 214 | 55.27 |
| 1.6107 | 20 | 125 | 57.14 |
| 1.5547 | 12 | 300 | 59.40 |
| 1.5087 | 6 | 0·2·10 | 61.40 |
| 1.4960 | 1 | 217 | 61.98 |
| 1.4360 | <1 | 128 | 64.88 |
| 1.4243 | <1 | 2·0·11 | 65.48 |
| 1.4066 | 1 | 306,1·1·12 | 66.41 |
| 1.3521 | 3 | 0·1·14 | 69.46 |
| 1.3468 | 10 | 220 | 69.77 |
| 1.3162 | 12 | 2·1·10 | 71.64 |
| 1.2913 | <1 | 131 | 73.24 |
| 1.2827 | <1 | 312 | 73.81 |
| 1.2746 | <1 | 0·2·13 | 74.36 |
| 1.2697 | 2 | 309 | 74.70 |
| 1.2517 | 1 | 134 | 75.96 |
| 1.2298 | 7 | 315 | 77.56 |
| 1.2087 | 1 | 2·0·14 | 79.18 |
| 1.1844 | 8 | 1·1·15 | 81.14 |
| 1.1643 | <1 | 401 | 82.84 |
| 1.1583 | <1 | 042 | 83.37 |
| 1.1484 | 3 | 229 | 84.25 |
| 1.1353 | <1 | 404 | 85.45 |
| 1.1288 | <1 | 0·1·17 | 86.06 |
| 1.1188 | 3 | 045 | 87.02 |
| 1.1026 | 2 | 1·2·14 | 88.63 |
| 1.0828 | 4 | 1·3·10 | 90.69 |
| 1.0461 | <1 | 324 | 94.84 |
| 1.0333 | 5 | 235 | 96.40 |
| 1.0182 | 4 | 410 | 98.32 |

Strontium phosphate, alpha $\text{Sr}_3(\text{PO}_4)_2$ - continued

| $d (\text{\AA})$ | I | hkl | $2\phi (\text{)}^\circ$ |
|------------------|-----|-------------|-------------------------|
| 1.0161 | 3 | 1·0·19 | 98.59 |
| 1.0057 | 4 | 3·0·15 | 99.98 |
| 1.0049 | 2 | 4·0·10 | 100.09 |
| 0.9822 | <1 | 238 | 103.30 |
| .9784 | <1 | 0·4·11 | 103.86 |
| | | | |
| .9728 | <1 | 416 | 104.71 |
| .9711 | <1 | 1·2·17 | 104.97 |
| .9675 | 1 | 0·1·20 | 105.53 |
| .9542 | 1 | 3·1·14 | 107.66 |
| .9508 | 1 | 0·2·19 | 108.22 |
| | | | |
| .9422 | 3 | 2·2·15 | 109.68 |
| .9414 | 3 | 3·2·10 | 109.82 |
| .9237 | 1 | 419 | 113.00 |
| .9170 | <1 | 054 | 114.29 |
| .9105 | <1 | 2·0·20 | 115.55 |
| | | | |
| .9081 | 1 | 505 | 116.04 |
| .8994 | 1 | 0·4·14 | 117.83 |
| .8978 | 1 | 330 | 118.18 |
| .8964 | 2 | 2·1·19 | 118.47 |
| .8891 | <1 | 1·1·21 | 120.07 |
| | | | |
| .8828 | <1 | 1·0·22 | 121.50 |
| .8782 | <1 | 422 | 122.59 |
| .8680 | <1 | 244 | 125.11 |
| .8661 | <1 | 336, 4·1·12 | 125.59 |
| .8626 | 2 | 1·2·20 | 126.51 |
| | | | |
| .8605 | 4 | 425 | 127.05 |
| .8531 | 1 | 2·3·14 | 129.08 |
| .8438 | 1 | 0·5·10 | 131.80 |

Sucrose, C₁₂H₂₂O₁₁

Sample

The sample used was an NBS Standard Reference Material (Number 17)
moisture..... less than 0.01%
ash..... less than 0.01%
reducing substances... less than 0.02%

Color

Colorless

Optical data

Biaxial(-), N_α=1.540, N_β=1.558, N_γ=1.564; 2V is medium

Structure

Monoclinic, P2₁ (4), Z=2, structure determined by Beevers et al. [1952], and refined by Brown and Levy [1963].

NBS lattice constants:

a = 10.868(2) Å
b = 8.710(1)
c = 7.761(1)
β = 102.97(1)°

Density

(calculated) 1.588 g/cm³

Reference intensity

I/I_{corundum} = 0.7

Additional patterns

1. PDF card 6-0142 [Palmer, Agriculture Res. Service, Albany, California]

References

Brown, G.M. and Levy, H.A. (1963). Science 141, 921.
Beevers, C.A., McDonald, T.R.R., Robertson, J.H., and Stern, F. (1952). Acta Cryst. 5, 689.

| Internal standard W, a = 3.16516 Å ° CuKα ₁ , λ = 1.54056 Å; temp. 25 °C | | | |
|--|-----|----------|-------|
| d (Å) | I | hkl | 2θ(°) |
| 10.59 | 14 | 100 | 8.34 |
| 7.58 | 65 | 001 | 11.67 |
| 6.94 | 40 | 101 | 12.74 |
| 6.73 | 55 | 110 | 13.14 |
| 5.712 | 30 | 011 | 15.50 |
| 5.424 | 11 | 111 | 16.33 |
| 5.298 | 14 | 200 | 16.72 |
| 4.884 | 12 | 201 | 18.15 |
| 4.706 | 100 | 111 | 18.84 |
| 4.523 | 80 | 210 | 19.61 |
| 4.354 | 25 | 020 | 20.38 |
| 4.259 | 30 | 211 | 20.84 |
| 4.028 | 30 | 120 | 22.05 |
| 3.943 | 11 | 201 | 22.53 |
| 3.776 | 18 | 002,021 | 23.54 |
| 3.690 | 8 | 121 | 24.10 |
| 3.591 | 100 | 211 | 24.77 |
| 3.531 | 45 | 300 | 25.20 |
| 3.467 | 3 | 012,202 | 25.67 |
| 3.437 | 5 | 121 | 25.90 |
| 3.364 | 11 | 220 | 26.47 |
| 3.272 | 5 | 310 | 27.23 |
| 3.254 | 10 | 221 | 27.39 |
| 3.222 | 7 | 212 | 27.66 |
| 3.112 | 9 | 112 | 28.66 |
| 2.956 | 2 | 301 | 30.21 |
| 2.923 | 6 | 221 | 30.56 |
| 2.882 | 25 | 122 | 31.00 |
| 2.856 | 6 | 022 | 31.29 |
| 2.799 | 20 | 130,311+ | 31.95 |
| 2.777 | 4 | 312 | 32.21 |
| 2.742 | 10 | 320 | 32.63 |
| 2.711 | 4 | 222,031 | 33.01 |
| 2.677 | 10 | 131 | 33.44 |
| 2.661 | 4 | 212 | 33.65 |
| 2.648 | 2 | 400,122 | 33.82 |
| 2.586 | 5 | 103 | 34.66 |
| 2.574 | 4 | 131,411 | 34.82 |
| 2.545 | 3 | 230 | 35.24 |
| 2.521 | 5 | 003 | 35.58 |
| 2.504 | 6 | 203 | 35.83 |
| 2.496 | 7 | 231 | 35.95 |
| 2.479 | 9 | 113 | 36.20 |
| 2.444 | 5 | 321 | 36.74 |
| 2.430 | 6 | 322 | 36.96 |
| 2.406 | 9 | 213 | 37.34 |
| 2.349 | 40 | 222,412 | 38.28 |
| 2.339 | 16 | 401,231+ | 38.46 |
| 2.312 | 7 | 303 | 38.92 |
| 2.291 | 4 | 421 | 39.30 |

Sucrose, C₁₂H₂₂O₁₁ - continued

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | <i>2θ</i> (°) |
|--------------|----------|------------|---------------|
| 2.258 | 14 | 113 | 39.89 |
| 2.253 | 11 | 312 | 39.98 |
| 2.234 | 10 | 313 | 40.33 |
| 2.189 | 5 | 132 | 41.20 |
| 2.171 | 5 | 223, 501 | 41.57 |
| 2.133 | 1 | 140 | 42.34 |
| 2.101 | 2 | 203 | 43.02 |
| 2.091 | 2 | 041 | 43.23 |
| 2.075 | 7 | 141, 403 | 43.58 |
| 2.060 | 6 | 123, 510 | 43.92 |
| 2.042 | 10 | 213, 323 | 44.33 |
| 2.028 | 4 | 141 | 44.64 |
| 2.014 | 1 | 240, 232 | 44.97 |
| 2.000 | 1 | 512 | 45.30 |
| 1.971 | 1 | 402 | 46.00 |
| 1.956 | 4 | 430 | 46.39 |
| 1.942 | 3 | 521 | 46.74 |
| 1.929 | 5 | 133, 501 | 47.07 |
| 1.924 | 5 | 204, 412 | 47.21 |
| 1.904 | 6 | 520, 033 | 47.72 |
| 1.895 | 4 | 233, 142 | 47.96 |
| 1.887 | 4 | 042 | 48.18 |
| 1.885 | 3 | 511 | 48.23 |
| 1.870 | 2 | 432 | 48.66 |
| 1.855 | 3 | 340 | 49.08 |
| 1.823 | 3 | 142, 313+ | 50.00 |
| 1.818 | 1 | 332 | 50.13 |
| 1.809 | 3 | 333, 314 | 50.41 |
| 1.795 | 5 | 422 | 50.81 |
| 1.773 | <1 | 611 | 51.50 |
| 1.764 | 2 | 600, 521 | 51.79 |
| 1.753 | 2 | 341 | 52.12 |
| 1.733 | 2 | 024, 404 | 52.79 |
| 1.718 | 1 | 150, 242 | 53.27 |
| 1.698 | 4 | 051 | 53.97 |
| 1.693 | 5 | 441, 502+ | 54.13 |
| 1.672 | 2 | 621 | 54.87 |
| 1.658 | 2 | 124 | 55.37 |
| 1.638 | 3 | 214 | 56.12 |
| 1.635 | 2 | 620 | 56.21 |

Zinc ammine bromide, $\text{Zn}(\text{NH}_3)_2\text{Br}_2$

Sample

The sample was made by dissolving Zn in hydro-bromic acid and adding NH_4Br and NH_4OH .

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.650$, $N_\gamma = 1.712$

Structure

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

NBS lattice constants:

$a = 8.419(1)$

$b = 8.816(1)$

$c = 8.122(1)$

Density

(calculated) 2.856 g/cm^3

Reference intensity

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

References

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

| $d (\text{\AA})$ | I | Internal standard W, $a = 3.16516 \text{ \AA}$ | |
|------------------|-----|--|--------------------------|
| | | hkl | $2\beta (\text{^\circ})$ |
| 6.08 | 30 | 110 | 14.55 |
| 5.973 | 35 | 011 | 14.82 |
| 4.410 | 55 | 020 | 20.12 |
| 4.209 | 13 | 200 | 21.09 |
| 4.062 | 95 | 002 | 21.86 |
| 3.521 | 25 | 121 | 25.27 |
| 3.441 | 19 | 211 | 25.82 |
| 3.377 | 19 | 112 | 26.37 |
| 3.044 | 50 | 220 | 29.32 |
| 2.986 | 100 | 022 | 29.90 |
| 2.922 | 13 | 202 | 30.57 |
| 2.773 | 3 | 130 | 32.26 |
| 2.764 | 4 | 031 | 32.36 |
| 2.436 | 20 | 222 | 36.87 |
| 2.309 | 11 | 231 | 38.97 |
| 2.292 | 6 | 132 | 39.28 |
| 2.272 | 5 | 321 | 39.63 |
| 2.225 | 7 | 123 | 40.50 |
| 2.205 | 7 | 213,040 | 40.89 |
| 2.105 | 7 | 400 | 42.93 |
| 2.062 | 2 | 141 | 43.87 |
| 2.030 | 16 | 004,330 | 44.59 |
| 1.986 | 1 | 411 | 45.65 |
| 1.953 | 10 | 240 | 46.46 |
| 1.937 | 2 | 042 | 46.87 |
| 1.926 | 3 | 114 | 47.14 |
| 1.899 | 3 | 420 | 47.85 |
| 1.869 | 5 | 402 | 48.69 |
| 1.844 | 6 | 024 | 49.37 |
| 1.829 | 2 | 204 | 49.82 |
| 1.815 | 4 | 332 | 50.20 |
| 1.799 | 6 | 233 | 50.69 |
| 1.782 | 3 | 323 | 51.23 |
| 1.759 | 19 | 242 | 51.93 |
| 1.722 | 10 | 051 | 53.13 |
| 1.689 | 8 | 224 | 54.26 |
| 1.674 | 1 | 431,143 | 54.78 |
| 1.596 | 2 | 251 | 57.72 |
| 1.5320 | 2 | 512 | 60.37 |
| 1.4994 | 3 | 125 | 61.80 |
| 1.4936 | 4 | 251,044,+ | 62.09 |
| 1.4774 | 5 | 053 | 62.85 |
| 1.4611 | 2 | 053,404 | 63.63 |
| 1.4356 | 1 | 334 | 64.90 |
| 1.4256 | 2 | 442,161 | 65.41 |
| 1.4075 | 5 | 244 | 66.36 |
| 1.3870 | 2 | 424,260 | 67.47 |
| 1.3821 | 3 | 062 | 67.74 |
| 1.3534 | 2 | 006 | 69.38 |

Zinc fluoride hydrate, $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$

Sample

The sample was prepared by slow evaporation, at room temperature, of an aqueous solution of ZnF_2 .

Color

Colorless

Optical data

Biaxial (-), $N_\alpha = 1.460$, $N_\beta = 1.458$, $N_\gamma = 1.448$; 2V is medium.

Structure

Orthorhombic, $P2_1ab$ (29), $Z=4$, isostructural with $\text{NiF}_2 \cdot 4\text{H}_2\text{O}$ [Rao et al., 1965].

NBS lattice constants:

$$\begin{aligned} a &= 7.544(2)\text{\AA} \\ b &= 12.641(2) \\ c &= 5.292(1) \end{aligned}$$

Density
(calculated) 2.309 g/cm^3

Reference intensity

$$I/I_{\text{corundum}} = 2.3$$

Polymorphism

Easwaran and Srinivasan [1965] found by comparison of powder patterns that $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ was isostructural with $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$. However, Penfold and Taylor [1960] reported $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ as rhombohedral. This suggests a second form of $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ exists.

References

- Easwaran, K.R.K. and Srinivasan, R. (1965). Proc. Nuclear Physics - Solid State Physics Symposium, Calcutta, Part A, 171.
- Penfold, B.R. and Taylor, M.R. (1960). Acta Cryst. **13**, 953.
- Rao, K.V.K., Naidu, S.V.N., and Rao, P.V. (1965). Indian J. Pure Applied Phys. **3**, 68.

| Internal standard Ag, $a = 4.08641 \text{ \AA}$ $\text{CuK}\alpha_1, \lambda = 1.54056 \text{ \AA}; \text{ temp. } 25^\circ\text{C}$ | | | |
|---|-----|-------|---------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
| 5.29 | 6 | 001 | 16.73 |
| 4.87 | 100 | 011 | 18.19 |
| 4.844 | 100 | 120 | 18.30 |
| 4.098 | 70 | 111 | 21.67 |
| 3.776 | 7 | 200 | 23.54 |

| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ |
|------------------|-----|---------|---------------------------|
| 3.577 | 5 | 121 | 24.87 |
| 3.297 | 6 | 031 | 27.02 |
| 3.160 | 25 | 040 | 28.22 |
| 3.072 | 4 | 201 | 29.04 |
| 3.023 | 9 | 131 | 29.52 |
| 2.985 | 40 | 211 | 29.91 |
| 2.762 | 20 | 221 | 32.39 |
| 2.592 | 10 | 012 | 34.58 |
| 2.555 | 12 | 141 | 35.10 |
| 2.484 | 3 | 231 | 36.13 |
| 2.449 | 6 | 112 | 36.67 |
| 2.323 | 10 | 122 | 38.73 |
| 2.281 | 4 | 051 | 39.47 |
| 2.236 | 14 | 311 | 40.30 |
| 2.202 | 3 | 241 | 40.96 |
| 2.184 | 14 | 151 | 41.31 |
| 2.167 | 16 | 202 | 41.65 |
| 2.148 | 3 | 132 | 42.02 |
| 2.135 | 4 | 212 | 42.29 |
| 2.029 | 16 | 160,042 | 44.62 |
| 1.999 | 4 | 331 | 45.32 |
| 1.957 | 4 | 061 | 46.35 |
| 1.952 | 8 | 251 | 46.49 |
| 1.927 | 4 | 232 | 47.13 |
| 1.887 | 8 | 400 | 48.19 |
| 1.845 | 2 | 341 | 49.36 |
| 1.804 | 6 | 312 | 50.54 |
| 1.786 | 12 | 242 | 51.09 |
| 1.759 | 13 | 411 | 51.94 |
| 1.751 | 18 | 322 | 52.20 |
| 1.738 | 8 | 261 | 52.63 |
| 1.709 | 4 | 071 | 53.59 |
| 1.689 | 2 | 351 | 54.25 |
| 1.673 | 2 | 332 | 54.84 |
| 1.667 | 4 | 171 | 55.06 |
| 1.658 | 4 | 123 | 55.36 |
| 1.644 | 4 | 252 | 55.88 |
| 1.619 | 3 | 440 | 56.83 |
| 1.615 | 5 | 360 | 56.97 |
| 1.610 | 5 | 162 | 57.18 |
| 1.589 | 2 | 133 | 57.96 |
| 1.581 | 2 | 080 | 58.32 |
| 1.579 | 2 | 342 | 58.41 |
| 1.557 | 2 | 271 | 59.29 |
| 1.544 | 1 | 361 | 59.85 |
| 1.541 | 3 | 043 | 60.02 |
| 1.537 | 1 | 402 | 60.19 |
| 1.4934 | 5 | 233 | 62.10 |
| 1.4671 | 5 | 520 | 63.34 |

Additional patterns

1. PDF card 1-253 [New Jersey Zinc Co.]

Calcium bromide, CaBr_2

Structure

Orthorhombic, Pnnm (58), $Z=2$. The structure was determined by Döll and Klemm [1939], and refined by Brackett et al. [1963]. It is isostructural with CaCl_2 [van Bever and Nieuwenkamp, 1935].

Lattice parameters

$a=6.584(6)$, $b=6.871(6)$, $c=4.342(4)\text{\AA}$ [Brackett et al., 1963].

Density

(calculated) 3.380 g/cm^3

Thermal parameters

Isotropic, overall $B=1.0$

Scattering factors

Ca^{2+} [International Tables, 1962]
 Br^- [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 2.474×10^4

Additional patterns

1. PDF card 2-535 [Döll and Klemm, 1939]

Reference

- van Bever, A.K. and Nieuwenkamp, W. (1935). Z. Krist. 90, 374.
- Brackett, E.B., Brackett, T.E., and Sass, R.L. (1963). J. Inorg. Nucl. Chem. 25, 1295.
- Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
- Döll, W. and Klemm, W. (1939). Z. anorg.u.allgem. Chem. 241, 233.
- International Tables for X-ray Crystallography III (1962), 204.

| $d (\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | $2\theta (\text{ }^\circ)$ $\lambda = 1.54056 \text{\AA}$ |
|------------------|-----|-----------------------------------|-----|-----|--|
| | | h | k | l | |
| 4.75 | 20 | 1 | 1 | 0 | 18.66 |
| 3.672 | 9 | 0 | 1 | 1 | 24.22 |
| 3.625 | 3 | 1 | 0 | 1 | 24.54 |
| 3.435 | 1 | 0 | 2 | 0 | 25.92 |
| 3.292 | 21 | 2 | 0 | 0 | 27.06 |
| 3.206 | 100 | 1 | 1 | 1 | 27.80 |
| 3.046 | 52 | 1 | 2 | 0 | 29.30 |
| 2.968 | 1 | 2 | 1 | 0 | 30.08 |
| 2.494 | 5 | 1 | 2 | 1 | 35.98 |
| 2.451 | 38 | 2 | 1 | 1 | 36.64 |
| 2.377 | 12 | 2 | 2 | 0 | 37.82 |
| 2.171 | 15 | 0 | 0 | 2 | 41.56 |
| 2.085 | 1 | 2 | 2 | 1 | 43.36 |
| 2.026 | 23 | 0 | 3 | 1 | 44.70 |
| 1.975 | 2 | 1 | 1 | 2 | 45.92 |
| 1.958 | 3 | 3 | 0 | 1 | 46.32 |
| 1.883 | 15 | 3 | 1 | 1 | 48.28 |
| 1.850 | 8 | 3 | 2 | 0 | 49.22 |
| 1.812 | 5 | 2 | 0 | 2 | 50.30 |
| 1.768 | 15 | 1 | 2 | 2 | 51.66 |
| 1.725 | 8 | 2 | 3 | 1 | 53.04 |
| 1.662 | 4 | 1 | 4 | 0 | 55.22 |
| 1.646 | 5 | 4 | 0 | 0 | 55.80 |
| 1.603 | 5 | 2 | 2 | 2 | 57.44 |
| 1.585 | 1 | 3 | 3 | 0 | 58.16 |
| 1.552 | 1 | 1 | 4 | 1 | 59.50 |
| 1.523 | 4 | 2 | 4 | 0 | 60.76 |
| 1.502 | 1 | 4 | 1 | 1 | 61.70 |
| 1.408 | 5 | 3 | 2 | 2 | 66.34 |
| 1.404 | 3 | 4 | 2 | 1 | 66.52 |
| 1.385 | 4 | 1 | 1 | 3 | 67.60 |
| 1.353 | 1 | 3 | 4 | 0 | 69.42 |
| 1.320 | 3 | 1 | 4 | 2 | 71.42 |
| 1.312 | 3 | 4 | 0 | 2 | 71.92 |
| 1.301 | 3 | 2 | 1 | 3 | 72.60 |
| 1.285 | 4 | 1 | 5 | 1 | 73.66 |
| 1.280 | 2 | 3 | 3 | 2 | 74.00 |
| 1.278 | 6 | 4 | 3 | 1 | 74.16 |
| 1.247 | 3 | 2 | 4 | 2 | 76.32 |
| 1.240 | 2 | 5 | 1 | 1 | 76.84 |
| 1.230 | 1 | 5 | 2 | 0 | 77.58 |
| 1.223 | 3 | 0 | 3 | 3 | 78.04 |
| 1.217 | 1 | 2 | 5 | 1 | 78.52 |
| 1.190 | 2 | 3 | 1 | 3 | 80.68 |
| 1.148 | 2 | 3 | 4 | 2 | 84.28 |
| 1.147 | 2 | 2 | 3 | 3 | 84.38 |
| 1.145 | 2 | 0 | 6 | 0 | 84.54 |
| 1.125 | 2 | 3 | 5 | 1 | 86.42 |
| 1.086 | 1 | 0 | 0 | 4 | 90.40 |
| 1.070 | 1 | 5 | 2 | 2 | 92.10 |

Calcium bromide, CaBr_2 – continued

| d (Å) | I | hkl | 2θ (°) | $\lambda = 1.54056 \text{ Å}$ |
|---------------------------------|-----|---------|---------------|-------------------------------|
| | | | ° | |
| 1.051 | 1 | 6 1 1 | 94.22 | |
| 1.022 | 1 | 1 2 4 | 97.76 | |
| 1.016 | 1 | 5 4 1 | 98.58 | |
| 1.013 | 1 | 0 6 2 | 99.00 | |
| .985 | 2 | 1 5 3 | 102.84 | |
| .982 | 2 | 4 3 3 | 103.34 | |
| .968 | 1 | 2 6 2 | 105.44 | |
| .964 | 1 | 5 1 3 + | 106.02 | |
| .942 | 1 | 5 4 2 + | 109.76 | |
| .940 | 1 | 4 6 0 | 110.06 | |
| .936 | 1 | 3 2 4 | 110.74 | |
| .929 | 1 | 5 5 1 | 112.06 | |
| .919 | 2 | 2 7 1 + | 113.84 | |
| .909 | 1 | 1 4 4 | 115.88 | |
| .907 | 1 | 3 5 3 + | 116.20 | |
| .906 | 1 | 4 0 4 | 116.42 | |
| .884 | 1 | 2 4 4 | 121.24 | |
| .863 | 1 | 4 6 2 | 126.48 | |
| .854 | 1 | 1 1 5 | 128.76 | |
| .852 | 1 | 1 8 0 | 129.50 | |
| .851 | 1 | 6 4 2 | 129.74 | |
| .814 | 1 | 5 2 4 | 142.38 | |
| .812 | 1 | 0 3 5 | 143.12 | |
| .808 | 1 | 7 3 2 | 145.02 | |
| .802 | 1 | 3 1 5 | 147.68 | |
| .800 | 1 | 3 8 0 | 148.76 | |
| .795 | 1 | 5 5 3 | 151.56 | |
| .793 | 1 | 1 8 2 | 152.62 | |
| .789 | 2 | 2 7 3 + | 155.20 | |
| .788 | 1 | 0 6 4 | 155.78 | |
| .787 | 1 | 8 2 1 + | 156.52 | |
| Calculated Pattern (Integrated) | | | | |
| d (Å) | I | hkl | 2θ (°) | $\lambda = 1.54056 \text{ Å}$ |
| 4.75 | 18 | 1 1 0 | 18.65 | |
| 3.671 | 9 | 0 1 1 | 24.23 | |
| 3.625 | 3 | 1 0 1 | 24.54 | |
| 3.435 | 1 | 0 2 0 | 25.91 | |
| 3.292 | 20 | 2 0 0 | 27.06 | |
| 3.206 | 100 | 1 1 1 | 27.80 | |
| 3.046 | 51 | 1 2 0 | 29.30 | |
| 2.969 | 1 | 2 1 0 | 30.08 | |
| 2.493 | 6 | 1 2 1 | 35.99 | |
| 2.451 | 41 | 2 1 1 | 36.64 | |
| 2.377 | 13 | 2 2 0 | 37.82 | |
| 2.171 | 17 | 0 0 2 | 41.56 | |
| 2.085 | 1 | 2 2 1 | 43.36 | |
| 2.026 | 27 | 0 3 1 | 44.70 | |
| 1.975 | 3 | 1 1 2 | 45.92 | |
| 1.959 | 4 | 3 0 1 | 46.32 | |
| 1.936 | 1 | 1 3 1 | 46.89 | |
| 1.884 | 18 | 3 1 1 | 48.28 | |
| 1.850 | 10 | 3 2 0 | 49.23 | |
| 1.812 | 7 | 2 0 2 | 50.30 | |
| 1.768 | 18 | 1 2 2 | 51.66 | |
| 1.725 | 11 | 2 3 1 | 53.03 | |
| 1.718 | 1 | 0 4 0 | 53.29 | |
| 1.662 | 5 | 1 4 0 | 55.22 | |
| 1.646 | 6 | 4 0 0 | 55.81 | |
| 1.603 | 5 | 2 2 2 | 57.44 | |
| 1.585 | 2 | 3 3 0 | 58.17 | |
| 1.552 | 1 | 1 4 1 | 59.50 | |
| 1.523 | 5 | 2 4 0 | 60.77 | |
| 1.502 | 1 | 4 1 1 | 61.71 | |
| 1.408 | 7 | 3 2 2 | 66.34 | |
| 1.405 | 1 | 4 2 1 | 66.51 | |
| 1.385 | 6 | 1 1 3 | 67.60 | |
| 1.353 | 2 | 3 4 0 | 69.42 | |
| 1.347 | 1 | 0 4 2 | 69.75 | |
| 1.320 | 4 | 1 4 2 | 71.42 | |
| 1.312 | 5 | 4 0 2 | 71.93 | |
| 1.301 | 4 | 2 1 3 | 72.61 | |
| 1.285 | 6 | 1 5 1 | 73.66 | |
| 1.280 | 1 | 3 3 2 | 74.00 | |
| 1.277 | 9 | 4 3 1 | 74.17 | |
| 1.247 | 5 | 2 4 2 | 76.32 | |
| 1.239 | 3 | 5 1 1 | 76.85 | |
| 1.230 | 2 | 5 2 0 | 77.58 | |
| 1.224 | 4 | 0 3 3 | 78.04 | |
| 1.217 | 1 | 2 5 1 | 78.51 | |
| 1.190 | 3 | 3 1 3 | 80.68 | |
| 1.183 | 1 | 5 2 1 | 81.25 | |
| 1.148 | 2 | 3 4 2 | 84.28 | |
| 1.147 | 2 | 2 3 3 | 84.39 | |

Calcium bromide, CaBr_2 – continued

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ | d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|-------|--|---------|-----|-------|--|
| 1.145 | 2 | 0 6 0 | 84.54 | .806 | 1 | 1 7 3 | 145.64 |
| 1.125 | 4 | 3 5 1 | 86.43 | .802 | 3 | 3 1 5 | 147.68 |
| 1.111 | 1 | 5 1 2 | 87.78 | .800 | 2 | 3 8 0 | 148.76 |
| 1.086 | 1 | 0 0 4 | 90.41 | .798 | 1 | 6 5 2 | 149.96 |
| 1.082 | 1 | 2 6 0 | 90.82 | .795 | 3 | 5 5 3 | 151.55 |
| 1.070 | 2 | 5 2 2 | 92.10 | .793 | 4 | 1 8 2 | 152.60 |
| 1.051 | 2 | 6 1 1 | 94.22 | .792 | 1 | 6 6 0 | 152.92 |
| 1.045 | 1 | 5 4 0 | 94.96 | .789 | 5 | 2 7 3 | 155.18 |
| 1.031 | 1 | 2 0 4 | 96.70 | .789 | 2 | 7 0 3 | 155.21 |
| 1.022 | 3 | 1 2 4 | 97.76 | .788 | 3 | 2 3 5 | 155.41 |
| 1.016 | 1 | 5 4 1 | 98.60 | .788 | 4 | 0 6 4 | 155.78 |
| 1.013 | 2 | 0 6 2 | 99.01 | .787 | 2 | 8 2 1 | 156.27 |
| .987 | 1 | 2 2 4 | 102.54 | .787 | 1 | 5 7 0 | 156.35 |
| .985 | 3 | 1 5 3 | 102.84 | .784 | 3 | 7 1 3 | 158.90 |
| .982 | 4 | 4 3 3 | 103.34 | | | | |
| .968 | 1 | 2 6 2 | 105.44 | | | | |
| .965 | 1 | 0 3 1 | 105.94 | | | | |
| .964 | 2 | 5 1 3 | 106.02 | | | | |
| .947 | 1 | 1 7 1 | 108.78 | | | | |
| .942 | 1 | 6 2 2 | 109.74 | | | | |
| .942 | 1 | 5 4 2 | 109.77 | | | | |
| .940 | 2 | 4 6 0 | 110.05 | | | | |
| .936 | 2 | 3 2 4 | 110.73 | | | | |
| .929 | 2 | 5 5 1 | 112.07 | | | | |
| .925 | 1 | 6 4 0 | 112.81 | | | | |
| .919 | 3 | 2 7 1 | 113.83 | | | | |
| .919 | 1 | 7 0 1 | 113.85 | | | | |
| .911 | 1 | 7 1 1 | 115.43 | | | | |
| .909 | 1 | 1 4 4 | 115.89 | | | | |
| .907 | 2 | 3 5 3 | 116.18 | | | | |
| .907 | 1 | 7 2 0 | 116.22 | | | | |
| .906 | 2 | 4 0 4 | 116.43 | | | | |
| .884 | 2 | 2 4 4 | 121.25 | | | | |
| .878 | 1 | 3 7 1 | 122.75 | | | | |
| .870 | 1 | 7 3 0 | 124.58 | | | | |
| .867 | 1 | 0 1 3 | 125.25 | | | | |
| .863 | 3 | 4 6 2 | 126.49 | | | | |
| .854 | 2 | 1 1 5 | 128.76 | | | | |
| .852 | 1 | 1 8 0 | 129.50 | | | | |
| .851 | 2 | 6 4 2 | 129.75 | | | | |
| .847 | 1 | 5 4 3 | 130.77 | | | | |
| .847 | 1 | 3 4 4 | 130.97 | | | | |
| .837 | 2 | 7 2 2 | 133.92 | | | | |
| .833 | 2 | 2 1 5 | 135.09 | | | | |
| .828 | 1 | 4 7 1 | 137.10 | | | | |
| .823 | 1 | 8 0 0 | 138.76 | | | | |
| .817 | 1 | 6 3 3 | 141.10 | | | | |
| .814 | 2 | 5 2 4 | 142.37 | | | | |
| .812 | 3 | 0 3 5 | 143.11 | | | | |
| .808 | 2 | 7 3 2 | 145.02 | | | | |

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$

Structure

Triclinic, $P\bar{1}$ (2), $Z=2$. The structure was determined by Thewalt and Bugg [1973].

Lattice parameters

$a=6.593(2)$, $b=6.364(5)$, $c=8.557(3)\text{\AA}$, $\alpha=97.77(5)$,
 $\beta=93.52(4)$, $\gamma=110.56(3)^\circ$ [ibid.]

Density
 (calculated) 1.838 g/cm^3

Thermal parameters

Anisotropic [ibid.]

Polymorphism

Three crystalline forms have been described.
 [Gmelins Handbuch, 1957]. The form characterized here apparently corresponds to the α -form [Thewalt and Bugg, 1973]

Scattering factors

Ca^{2+} , Cl^- [Cromer and Waber, 1965], corrected for dispersion using terms $\Delta f'$ and $\Delta f''$ from Cromer and Liberman [1970].

Scale factor

(integrated intensities) 0.2942×10^4

Additional patterns

1. PDF card 1-1080 [Hanawalt et al., 1938]

Reference

- Cromer, D.T. and Liberman, D. (1970). J.Chem.Phys., 53, 1891.
- Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
- Gmelins Handbuch der Anorganischen Chemie.Calcium, Teil B (1957). Pg. 468.
- Hanawalt, J.D., Rinn, H.W., and Frevel, L.K.(1938) Ind. Eng. Chem. Anal. Ed. 10, 457.
- Thewalt, U. and Bugg, C.E. (1973). Acta Cryst.B29 615.

| $d (\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | $2\theta (^\circ)$ $\lambda = 1.54056 \text{\AA}$ |
|------------------|-----|-----------------------------------|-----|-----|--|
| | | h | k | l | |
| 6.13 | 51 | 1 | 0 | 0 | 14.44 |
| 5.87 | 91 | 0 | 1 | 0 | 15.08 |
| 5.31 | 29 | -1 | 1 | 0 | 16.68 |
| 5.25 | 27 | -1 | 0 | 1 + | 16.88 |
| 4.70 | 28 | 1 | 0 | 1 | 18.86 |
| 4.60 | 100 | 1 | -1 | 1 | 19.28 |
| 4.48 | 3 | 0 | 1 | 1 | 19.82 |
| 4.40 | 2 | -1 | 1 | 1 | 20.18 |
| 3.729 | 9 | 0 | -1 | 2 | 23.84 |
| 3.633 | 15 | 1 | 1 | 0 | 24.48 |
| 3.567 | 53 | -1 | -1 | 1 | 24.94 |
| 3.383 | 4 | 1 | -1 | 2 | 26.32 |
| 3.295 | 38 | 1 | 0 | 2 | 27.04 |
| 3.243 | 4 | -2 | 1 | 0 | 27.48 |
| 3.222 | 16 | -1 | 1 | 2 | 27.66 |
| 3.180 | 22 | 0 | 1 | 2 | 28.04 |
| 3.129 | 34 | -1 | 2 | 0 | 28.50 |
| 3.064 | 33 | 2 | 0 | 0 | 29.12 |
| 3.056 | 24 | 1 | -2 | 1 | 29.20 |
| 3.021 | 6 | -1 | -1 | 2 | 29.54 |
| 2.996 | 38 | 2 | -1 | 1 + | 29.80 |
| 2.938 | 62 | 0 | 2 | 0 | 30.40 |
| 2.930 | 42 | 0 | -2 | 1 | 30.48 |
| 2.826 | 31 | -1 | 2 | 1 | 31.64 |
| 2.806 | 23 | 0 | 0 | 3 | 31.86 |
| 2.778 | 4 | 2 | 0 | 1 | 32.20 |
| 2.715 | 71 | 0 | -1 | 3 | 32.96 |
| 2.667 | 9 | 1 | -2 | 2 | 33.58 |
| 2.657 | 22 | -2 | 2 | 0 | 33.70 |
| 2.629 | 74 | -2 | 0 | 2 + | 34.08 |
| 2.609 | 21 | -2 | 1 | 2 | 34.34 |
| 2.572 | 19 | 2 | -2 | 1 | 34.86 |
| 2.535 | 9 | 1 | -1 | 3 | 35.38 |
| 2.498 | 14 | -2 | 2 | 1 | 35.92 |
| 2.445 | 6 | 1 | 0 | 3 | 36.72 |
| 2.433 | 10 | -1 | 1 | 3 + | 36.92 |
| 2.398 | 29 | -2 | -1 | 1 | 37.48 |
| 2.382 | 65 | 0 | 1 | 3 + | 37.74 |
| 2.350 | 18 | 2 | 0 | 2 | 38.26 |
| 2.300 | 17 | 2 | -2 | 2 | 39.14 |
| 2.239 | 22 | 0 | 2 | 2 | 40.24 |
| 2.234 | 20 | -2 | -1 | 2 | 40.34 |
| 2.224 | 16 | 1 | -2 | 3 + | 40.52 |
| 2.219 | 30 | -1 | -2 | 2 | 40.62 |
| 2.205 | 62 | 2 | 1 | 1 + | 40.90 |
| 2.198 | 60 | -2 | 2 | 2 | 41.02 |
| 2.193 | 25 | -3 | 1 | 0 | 41.12 |
| 2.156 | 30 | -2 | 1 | 3 + | 41.86 |
| 2.105 | 8 | 0 | 0 | 4 + | 42.94 |
| 2.100 | 8 | -1 | 3 | 0 | 43.04 |

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ – continued

| d (Å) | I | hkl | $2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$ | d (Å) | I | hkl | $2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|-----------|--|---------|-----|-----------|--|
| 2.096 | 8 | 0 -1 4 | 43.12 | 1.555 | 2 | -2 0 5 | 59.38 |
| 2.090 | 26 | 2 -1 3 | 43.26 | 1.551 | 2 | 0 1 5 | 59.54 |
| 2.066 | 16 | -1 0 4 + | 43.78 | 1.541 | 3 | 1 -4 2 | 59.96 |
| 2.055 | 6 | 1 1 3 | 44.02 | 1.533 | 3 | 3 -3 3 + | 60.34 |
| 2.041 | 6 | -3 0 1 | 44.34 | 1.514 | 1 | -2 1 5 | 61.16 |
| 2.004 | 30 | 2 -3 1 + | 45.20 | 1.506 | 1 | -2 4 1 | 61.52 |
| 1.999 | 18 | -3 1 2 | 45.34 | 1.498 | 5 | -4 0 2 | 61.90 |
| 1.994 | 6 | 1 -3 2 | 45.46 | 1.493 | 10 | -2 -1 5 + | 62.14 |
| 1.980 | 6 | 2 -2 3 + | 45.80 | 1.484 | 3 | 1 3 2 + | 62.54 |
| 1.974 | 13 | -1 3 1 + | 45.94 | 1.481 | 3 | 4 -3 1 | 62.70 |
| 1.958 | 6 | 0 3 0 + | 46.32 | 1.474 | 3 | 3 -2 4 + | 63.02 |
| 1.934 | 1 | 3 0 1 | 46.94 | 1.468 | 8 | 0 4 0 | 63.28 |
| 1.919 | 7 | -2 3 1 | 47.32 | 1.465 | 6 | -3 3 3 + | 63.44 |
| 1.901 | 6 | 0 -3 2 | 47.80 | 1.454 | 1 | -3 -1 4 | 63.98 |
| 1.897 | 4 | 3 -1 2 | 47.92 | 1.452 | 1 | -1 -3 4 | 64.06 |
| 1.883 | 2 | 0 1 4 | 48.28 | 1.446 | 2 | -3 -2 2 | 64.40 |
| 1.878 | 3 | 0 2 3 | 48.42 | 1.442 | 3 | 1 2 4 | 64.58 |
| 1.865 | 1 | 0 -2 4 | 48.78 | 1.436 | 1 | 1 1 5 | 64.88 |
| 1.851 | 3 | 1 -2 4 | 49.18 | 1.431 | 2 | -3 4 1 + | 65.14 |
| 1.843 | 3 | -2 -2 1 | 49.42 | 1.428 | 3 | 3 -4 2 | 65.28 |
| 1.838 | 2 | -2 0 4 | 49.54 | 1.424 | 3 | -4 2 3 | 65.48 |
| 1.817 | 5 | 2 2 0 | 50.18 | 1.420 | 4 | 0 -1 6 | 65.70 |
| 1.784 | 5 | -2 -2 2 + | 51.16 | 1.417 | 3 | -4 0 3 + | 65.88 |
| 1.759 | 6 | 3 0 2 | 51.94 | 1.414 | 5 | 1 -3 5 + | 66.04 |
| 1.754 | 7 | -2 3 2 + | 52.10 | 1.407 | 4 | -4 3 2 + | 66.36 |
| 1.750 | 16 | 0 -3 3 | 52.24 | 1.403 | 6 | 0 0 6 + | 66.58 |
| 1.745 | 9 | 3 1 0 | 52.40 | 1.391 | 7 | -2 2 5 + | 67.24 |
| 1.720 | 1 | -1 -3 1 | 53.20 | 1.377 | 2 | -2 -3 3 + | 68.00 |
| 1.716 | 4 | 2 2 1 | 53.36 | 1.367 | 4 | 4 -1 3 + | 68.60 |
| 1.696 | 5 | 0 -1 5 + | 54.04 | 1.358 | 7 | -2 -2 5 + | 69.12 |
| 1.691 | 8 | 2 -2 4 + | 54.18 | 1.355 | 5 | -3 4 2 | 69.30 |
| 1.679 | 4 | -1 -3 2 | 54.60 | 1.344 | 3 | -4 1 4 + | 69.96 |
| 1.675 | 3 | -1 0 5 | 54.76 | 1.340 | 2 | -1 1 6 | 70.16 |
| 1.672 | 2 | 0 3 2 | 54.88 | 1.334 | 1 | 2 -4 4 | 70.54 |
| 1.664 | 5 | -3 2 3 + | 55.14 | 1.331 | 2 | 4 -3 3 | 70.74 |
| 1.659 | 7 | 3 1 1 | 55.34 | 1.327 | 2 | 0 3 4 | 70.96 |
| 1.647 | 3 | 2 0 4 | 55.76 | 1.323 | 3 | 1 4 0 + | 71.20 |
| 1.635 | 7 | -4 1 0 | 56.20 | 1.317 | 1 | -1 -3 5 | 71.56 |
| 1.631 | 4 | -4 1 1 | 56.38 | 1.314 | 1 | -3 -1 5 | 71.80 |
| 1.622 | 9 | -4 2 0 | 56.70 | 1.311 | 1 | -1 -2 6 | 71.98 |
| 1.608 | 6 | 1 3 1 | 57.26 | 1.305 | 3 | -4 -1 3 + | 72.36 |
| 1.603 | 4 | -4 2 1 | 57.44 | 1.302 | 2 | -2 4 3 + | 72.54 |
| 1.592 | 2 | -3 -1 3 + | 57.88 | 1.297 | 1 | 3 -1 5 | 72.88 |
| 1.582 | 3 | 4 -1 1 + | 58.26 | 1.286 | 1 | -1 4 3 | 73.56 |
| 1.578 | 5 | 1 0 5 + | 58.42 | 1.283 | 4 | 2 1 5 | 73.82 |
| 1.572 | 4 | 2 2 2 | 58.70 | 1.271 | 1 | 2 2 4 | 74.64 |
| 1.567 | 3 | 3 0 3 | 58.88 | 1.267 | 1 | -5 3 0 | 74.90 |
| 1.564 | 3 | -2 4 0 | 59.00 | 1.255 | 1 | 1 -5 1 | 75.74 |
| 1.563 | 3 | -1 4 0 | 59.06 | 1.254 | 1 | 3 1 4 | 75.82 |
| 1.560 | 3 | -3 0 4 | 59.16 | | | | |

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ – continued

| Calculated Pattern (Integrated) | | | | d (\AA) | I | hkl | $2\theta(\text{ }^\circ)$ $\lambda = 1.54056 \text{\AA}$ | $2\theta(\text{ }^\circ)$ $\lambda = 1.54056 \text{\AA}$ |
|---------------------------------|-----|---------|--|----------------------|-------|-------|---|---|
| 6.13 | 46 | 1 0 0 | | 14.44 | 2.239 | 25 | 0 2 2 | 40.24 |
| 5.87 | 86 | 0 1 0 | | 15.07 | 2.234 | 18 | -2 -1 2 | 40.35 |
| 5.31 | 28 | -1 1 0 | | 16.67 | 2.225 | 10 | 1 -2 3 | 40.51 |
| 5.26 | 16 | -1 0 1 | | 16.85 | 2.224 | 2 | 0 -2 3 | 40.53 |
| 5.25 | 12 | 0 -1 1 | | 16.88 | 2.219 | 29 | -1 -2 2 | 40.63 |
| 4.70 | 28 | 1 0 1 | | 18.86 | 2.204 | 64 | 2 1 1 | 40.90 |
| 4.60 | 100 | 1 -1 1 | | 19.28 | 2.203 | 18 | -2 0 3 | 40.94 |
| 4.48 | 2 | 0 1 1 | | 19.81 | 2.198 | 32 | -2 2 2 | 41.03 |
| 4.40 | 2 | -1 1 1 | | 20.18 | 2.193 | 5 | -3 1 0 | 41.12 |
| 3.731 | 10 | 0 -1 2 | | 23.83 | 2.156 | 21 | -2 1 3 | 41.86 |
| 3.633 | 16 | 1 1 0 | | 24.48 | 2.156 | 3 | 1 2 1 | 41.86 |
| 3.568 | 57 | -1 -1 1 | | 24.94 | 2.156 | 14 | -3 1 1 | 41.87 |
| 3.383 | 4 | 1 -1 2 | | 26.32 | 2.107 | 1 | 1 -3 1 | 42.88 |
| 3.295 | 42 | 1 0 2 | | 27.04 | 2.105 | 9 | 0 0 4 | 42.93 |
| 3.244 | 4 | -2 1 0 | | 27.47 | 2.100 | 3 | -1 3 0 | 43.05 |
| 3.223 | 17 | -1 1 2 | | 27.66 | 2.096 | 5 | 0 -1 4 | 43.11 |
| 3.179 | 25 | 0 1 2 | | 28.05 | 2.090 | 32 | 2 -1 3 | 43.25 |
| 3.143 | 4 | 1 1 1 | | 28.37 | 2.067 | 14 | -1 0 4 | 43.76 |
| 3.129 | 37 | -1 2 0 | | 28.50 | 2.066 | 8 | -3 2 0 | 43.78 |
| 3.065 | 38 | 2 0 0 | | 29.11 | 2.055 | 7 | 1 1 3 | 44.02 |
| 3.054 | 7 | 1 -2 1 | | 29.22 | 2.041 | 6 | -3 0 1 | 44.33 |
| 3.021 | 5 | -1 -1 2 | | 29.54 | 2.006 | 4 | 3 -2 1 | 45.16 |
| 2.995 | 6 | -2 0 1 | | 29.80 | 2.004 | 37 | 2 -3 1 | 45.21 |
| 2.995 | 37 | 2 -1 1 | | 29.80 | 1.998 | 3 | -3 1 2 | 45.36 |
| 2.937 | 74 | 0 2 0 | | 30.41 | 1.993 | 3 | 1 -3 2 | 45.47 |
| 2.930 | 2 | 0 -2 1 | | 30.48 | 1.980 | 5 | 2 -2 3 | 45.79 |
| 2.825 | 35 | -1 2 1 | | 31.64 | 1.978 | 1 | -1 -2 3 | 45.83 |
| 2.807 | 24 | 0 0 3 | | 31.86 | 1.976 | 5 | -1 -1 4 | 45.89 |
| 2.777 | 4 | 2 0 1 | | 32.20 | 1.973 | 12 | -1 3 1 | 45.95 |
| 2.716 | 84 | 0 -1 3 | | 32.95 | 1.959 | 3 | 2 0 3 | 46.32 |
| 2.673 | 3 | -1 0 3 | | 33.49 | 1.958 | 5 | 0 3 0 | 46.33 |
| 2.667 | 6 | 1 -2 2 | | 33.57 | 1.934 | 2 | 3 0 1 | 46.93 |
| 2.657 | 22 | -2 2 0 | | 33.70 | 1.919 | 9 | -2 3 1 | 47.32 |
| 2.639 | 2 | 0 2 1 | | 33.94 | 1.902 | 7 | 0 -3 2 | 47.79 |
| 2.629 | 81 | -2 0 2 | | 34.07 | 1.896 | 1 | 3 -1 2 | 47.93 |
| 2.624 | 25 | 0 -2 2 | | 34.14 | 1.884 | 2 | 0 1 4 | 48.27 |
| 2.610 | 20 | -2 1 2 | | 34.33 | 1.878 | 3 | 0 2 3 | 48.43 |
| 2.571 | 22 | 2 -2 1 | | 34.86 | 1.866 | 1 | 0 -2 4 | 48.78 |
| 2.535 | 10 | 1 -1 3 | | 35.38 | 1.851 | 4 | 1 -2 4 | 49.17 |
| 2.499 | 17 | -2 2 1 | | 35.91 | 1.843 | 3 | -2 -2 1 | 49.42 |
| 2.446 | 7 | 1 0 3 | | 36.72 | 1.839 | 1 | -2 0 4 | 49.53 |
| 2.434 | 1 | -1 -1 3 | | 36.89 | 1.816 | 8 | 2 2 0 | 50.18 |
| 2.432 | 11 | -1 1 3 | | 36.93 | 1.784 | 7 | -2 -2 2 | 51.16 |
| 2.397 | 34 | -2 -1 1 | | 37.49 | 1.782 | 1 | -1 3 2 | 51.22 |
| 2.385 | 2 | 2 1 0 | | 37.68 | 1.759 | 7 | 3 0 2 | 51.94 |
| 2.382 | 73 | 0 1 3 | | 37.74 | 1.754 | 5 | -2 3 2 | 52.10 |
| 2.380 | 7 | -1 2 2 | | 37.78 | 1.753 | 1 | -3 0 3 | 52.14 |
| 2.350 | 21 | 2 0 2 | | 38.26 | 1.749 | 20 | 0 -3 3 | 52.24 |
| 2.338 | 1 | 1 2 0 | | 38.47 | 1.743 | 2 | 3 1 0 | 52.44 |
| 2.300 | 20 | 2 -2 2 | | 39.14 | 1.722 | 1 | -1 -3 1 | 53.14 |

Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ – continued

| d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ | d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ |
|----------------------|-----|---------|--|----------------------|-----|---------|--|
| 1.715 | 5 | 2 2 1 | 53.37 | 1.465 | 2 | -3 3 3 | 63.42 |
| 1.698 | 2 | 1 1 4 | 53.95 | 1.464 | 1 | -4 1 3 | 63.50 |
| 1.696 | 4 | 0 -1 5 | 54.03 | 1.454 | 1 | -3 -1 4 | 63.98 |
| 1.695 | 2 | 1 3 0 | 54.05 | 1.452 | 1 | -1 -3 4 | 64.06 |
| 1.692 | 8 | 2 -2 4 | 54.17 | 1.446 | 2 | -3 -2 2 | 64.40 |
| 1.689 | 1 | 2 1 3 | 54.25 | 1.442 | 4 | 1 2 4 | 64.59 |
| 1.679 | 5 | -1 -3 2 | 54.61 | 1.436 | 1 | 1 1 5 | 64.89 |
| 1.675 | 1 | -1 0 5 | 54.76 | 1.431 | 1 | 2 3 0 | 65.14 |
| 1.671 | 1 | 0 3 2 | 54.88 | 1.431 | 2 | -3 4 1 | 65.14 |
| 1.664 | 5 | -3 2 3 | 55.14 | 1.428 | 4 | 3 -4 2 | 65.28 |
| 1.663 | 1 | 3 -2 3 | 55.17 | 1.424 | 3 | -4 2 3 | 65.50 |
| 1.663 | 3 | 3 -3 2 | 55.19 | 1.420 | 5 | 0 -1 6 | 65.71 |
| 1.659 | 8 | 3 1 1 | 55.35 | 1.417 | 1 | 2 2 3 | 65.86 |
| 1.647 | 3 | 2 0 4 | 55.76 | 1.417 | 1 | -4 0 3 | 65.86 |
| 1.635 | 10 | -4 1 0 | 56.20 | 1.414 | 5 | 1 -3 5 | 66.04 |
| 1.629 | 1 | -4 1 1 | 56.43 | 1.413 | 3 | -2 4 2 | 66.09 |
| 1.622 | 14 | -4 2 0 | 56.71 | 1.408 | 2 | 2 0 5 | 66.34 |
| 1.607 | 8 | 1 3 1 | 57.26 | 1.407 | 4 | -4 3 2 | 66.38 |
| 1.602 | 1 | -4 2 1 | 57.48 | 1.403 | 7 | 0 0 6 | 66.58 |
| 1.592 | 3 | -3 -1 3 | 57.88 | 1.401 | 1 | 0 -4 3 | 66.69 |
| 1.589 | 1 | 0 2 4 | 57.98 | 1.392 | 4 | -1 3 4 | 67.17 |
| 1.583 | 1 | -1 1 5 | 58.25 | 1.391 | 9 | -2 2 5 | 67.23 |
| 1.582 | 2 | 4 -1 1 | 58.27 | 1.379 | 1 | -3 1 5 | 67.94 |
| 1.580 | 2 | 0 -2 5 | 58.37 | 1.377 | 3 | -2 -3 3 | 68.00 |
| 1.579 | 2 | 1 -4 1 | 58.39 | 1.367 | 6 | 4 -1 3 | 68.59 |
| 1.577 | 2 | 1 0 5 | 58.47 | 1.365 | 1 | 0 2 5 | 68.69 |
| 1.572 | 4 | 2 2 2 | 58.70 | 1.358 | 4 | -4 -1 2 | 69.09 |
| 1.567 | 1 | 3 0 3 | 58.90 | 1.358 | 1 | 0 -2 6 | 69.12 |
| 1.564 | 3 | -2 4 0 | 58.99 | 1.358 | 5 | -2 -2 5 | 69.13 |
| 1.563 | 1 | -1 4 0 | 59.07 | 1.358 | 3 | 2 -3 5 | 69.13 |
| 1.561 | 2 | -3 0 4 | 59.15 | 1.355 | 2 | -3 4 2 | 69.26 |
| 1.555 | 2 | -2 0 5 | 59.39 | 1.344 | 1 | -1 -4 1 | 69.93 |
| 1.551 | 1 | 0 1 5 | 59.54 | 1.343 | 4 | -4 1 4 | 69.97 |
| 1.542 | 4 | 1 -4 2 | 59.96 | 1.340 | 2 | -1 1 6 | 70.15 |
| 1.533 | 2 | 3 -3 3 | 60.32 | 1.334 | 1 | 2 -4 4 | 70.55 |
| 1.533 | 2 | 4 0 0 | 60.34 | 1.331 | 2 | 4 -3 3 | 70.74 |
| 1.514 | 1 | -2 1 5 | 61.15 | 1.327 | 2 | 0 3 4 | 70.97 |
| 1.506 | 1 | -2 4 1 | 61.51 | 1.323 | 2 | 1 4 0 | 71.19 |
| 1.498 | 4 | -4 0 2 | 61.90 | 1.323 | 1 | -3 3 4 | 71.20 |
| 1.498 | 2 | 4 -2 2 | 61.90 | 1.317 | 1 | -1 -3 5 | 71.56 |
| 1.493 | 7 | 0 3 3 | 62.13 | 1.314 | 1 | -3 -1 5 | 71.80 |
| 1.492 | 8 | -2 -1 5 | 62.15 | 1.311 | 1 | -1 -2 6 | 71.98 |
| 1.485 | 1 | 4 -1 2 | 62.47 | 1.305 | 2 | -4 2 4 | 72.36 |
| 1.484 | 4 | 1 3 2 | 62.55 | 1.305 | 2 | -4 -1 3 | 72.37 |
| 1.480 | 2 | 4 -3 1 | 62.70 | 1.303 | 1 | -2 1 6 | 72.48 |
| 1.478 | 1 | 4 0 1 | 62.84 | 1.302 | 1 | -2 4 3 | 72.53 |
| 1.476 | 1 | 2 -1 5 | 62.93 | 1.300 | 1 | -5 1 1 | 72.65 |
| 1.474 | 2 | 3 -2 4 | 63.01 | 1.297 | 1 | 3 -1 5 | 72.89 |
| 1.473 | 1 | 3 -1 4 | 63.07 | 1.286 | 1 | -1 4 3 | 73.56 |
| 1.469 | 12 | 0 4 0 | 63.27 | 1.283 | 5 | 2 1 5 | 73.82 |

Chromium chloride, CrCl₂

Structure

Orthorhombic, Pnnm (58), Z=2 [Handy and Gregory, 1951]. The structure was determined independently and practically at the same time in four different laboratories and reported jointly in one paper [Tracy et al., 1961]

Lattice parameters

a=6.631, b=5.980, c=3.487 Å [Tracy et al., 1961]

Density
(calculated) 2.952 g/cm³

Thermal parameters

Anisotropic; $\beta_{11}=0.0137$, $\beta_{22}=0.0119$ for all atoms

Atomic positions

Cr in 2a: 0,0,0
Cl in 4g: x,y,0 with x=0.360, y=0.275

Scattering factors

Cr²⁺, Cl⁻ [Berghuis et al., 1955]

Scale factor

(integrated intensities) 0.5267 x 10⁴

Additional patterns

1. PDF card 6-0159 [Handy and Gregory, 1951].
2. Oswald [1961]

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| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|-----|---|--|
| d (Å) | I | hkl | | 2θ(°) $\lambda = 1.54056 \text{ Å}$ |
| 4.44 | 100 | 1 | 1 | 0 |
| 3.314 | 8 | 2 | 0 | 0 |
| 3.011 | 15 | 0 | 1 | 1 |
| 2.990 | 2 | 0 | 2 | 0 |
| 2.899 | 36 | 2 | 1 | 0 |
| 2.743 | 41 | 1 | 1 | 1 |
| 2.230 | 19 | 2 | 1 | 1 |
| 2.220 | 15 | 2 | 2 | 0 |
| 2.147 | 49 | 1 | 2 | 1 |
| 2.073 | 4 | 3 | 1 | 0 |
| 1.909 | 2 | 1 | 3 | 0 |
| 1.873 | 2 | 2 | 2 | 1 |
| 1.867 | 18 | 3 | 0 | 1 |
| 1.782 | 2 | 3 | 1 | 1 |
| 1.743 | 10 | 0 | 0 | 2 |
| 1.731 | 8 | 0 | 3 | 1 |
| 1.708 | 3 | 2 | 3 | 0 |
| 1.674 | 4 | 1 | 3 | 1 |
| 1.623 | 6 | 1 | 1 | 2 |
| 1.543 | 1 | 2 | 0 | 2 |
| 1.534 | 3 | 2 | 3 | 1 |
| 1.494 | 8 | 2 | 1 | 2 + |
| 1.480 | 3 | 3 | 3 | 0 |
| 1.452 | 4 | 4 | 1 | 1 |
| 1.450 | 6 | 4 | 2 | 0 |
| 1.371 | 3 | 2 | 2 | 2 |
| 1.363 | 1 | 3 | 3 | 1 + |
| 1.334 | 1 | 3 | 1 | 2 |
| 1.269 | 1 | 2 | 4 | 1 |
| 1.240 | 1 | 5 | 0 | 1 |
| 1.220 | 2 | 2 | 3 | 2 |
| 1.214 | 1 | 5 | 1 | 1 |
| 1.177 | 1 | 1 | 5 | 0 |
| 1.167 | 3 | 3 | 4 | 1 |
| 1.135 | 2 | 0 | 4 | 2 |
| 1.128 | 2 | 3 | 3 | 2 |
| 1.125 | 2 | 1 | 1 | 3 |
| 1.115 | 3 | 4 | 2 | 2 |
| 1.079 | 1 | 2 | 1 | 3 |
| 1.071 | 1 | 2 | 5 | 1 |
| 1.069 | 3 | 1 | 2 | 3 |
| 1.029 | 2 | 3 | 0 | 3 |
| 1.004 | 1 | 0 | 3 | 3 |
| .976 | 1 | 1 | 5 | 2 |
| .934 | 1 | 4 | 5 | 1 |
| .933 | 1 | 6 | 0 | 2 |
| .933 | 1 | 5 | 3 | 2 |
| .874 | 1 | 7 | 2 | 1 + |
| .872 | 1 | 0 | 0 | 4 |
| .855 | 1 | 1 | 1 | 4 |
| .848 | 1 | 3 | 4 | 3 |
| .845 | 1 | 6 | 3 | 2 |

Chromium chloride, CrCl₂ – continued

| Calculated Pattern (Integrated) | | | |
|---------------------------------|-----|-------|------------------------|
| d (Å) | I | hkl | 2θ(°) λ = 1.54056 Å |
| 4.44 | 100 | 1 1 0 | 19.98 |
| 3.315 | 9 | 2 0 0 | 26.87 |
| 3.012 | 18 | 0 1 1 | 29.63 |
| 2.990 | 1 | 0 2 0 | 29.86 |
| 2.900 | 43 | 2 1 0 | 30.81 |
| 2.743 | 48 | 1 1 1 | 32.62 |
| 2.726 | 2 | 1 2 0 | 32.83 |
| 2.230 | 23 | 2 1 1 | 40.42 |
| 2.220 | 15 | 2 2 0 | 40.60 |
| 2.147 | 62 | 1 2 1 | 42.04 |
| 2.073 | 5 | 3 1 0 | 43.62 |
| 1.909 | 2 | 1 3 0 | 47.60 |
| 1.873 | 2 | 2 2 1 | 48.57 |
| 1.867 | 24 | 3 0 1 | 48.74 |
| 1.782 | 3 | 3 1 1 | 51.22 |
| 1.743 | 14 | 0 0 2 | 52.44 |
| 1.731 | 11 | 0 3 1 | 52.86 |
| 1.708 | 5 | 2 3 0 | 53.60 |
| 1.674 | 6 | 1 3 1 | 54.78 |
| 1.623 | 10 | 1 1 2 | 56.67 |
| 1.543 | 2 | 2 0 2 | 59.89 |
| 1.534 | 4 | 2 3 1 | 60.28 |
| 1.495 | 4 | 0 4 0 | 62.03 |
| 1.494 | 9 | 2 1 2 | 62.06 |
| 1.480 | 4 | 3 3 0 | 62.71 |
| 1.452 | 5 | 4 1 1 | 64.06 |
| 1.450 | 7 | 4 2 0 | 64.19 |
| 1.371 | 5 | 2 2 2 | 68.35 |
| 1.363 | 1 | 2 4 0 | 68.83 |
| 1.363 | 1 | 3 3 1 | 68.85 |
| 1.334 | 2 | 3 1 2 | 70.52 |
| 1.295 | 1 | 5 1 0 | 73.02 |
| 1.287 | 1 | 1 3 2 | 73.50 |
| 1.269 | 1 | 2 4 1 | 74.72 |
| 1.240 | 2 | 5 0 1 | 76.84 |
| 1.220 | 3 | 2 3 2 | 78.29 |
| 1.214 | 2 | 5 1 1 | 78.78 |
| 1.177 | 2 | 1 5 0 | 81.75 |
| 1.167 | 5 | 3 4 1 | 82.61 |
| 1.135 | 3 | 0 4 2 | 85.49 |
| 1.128 | 3 | 3 3 2 | 86.10 |
| 1.124 | 2 | 1 1 3 | 86.48 |
| 1.115 | 6 | 4 2 2 | 87.42 |
| 1.079 | 2 | 2 1 3 | 91.12 |
| 1.074 | 1 | 2 4 2 | 91.68 |
| 1.071 | 1 | 2 5 1 | 92.01 |
| 1.069 | 6 | 1 2 3 | 92.18 |
| 1.053 | 1 | 5 3 1 | 94.07 |
| 1.039 | 1 | 5 1 2 | 95.64 |
| 1.029 | 3 | 3 0 3 | 96.96 |

| d (Å) | I | hkl | 2θ(°) λ = 1.54056 Å |
|-------|---|-------|------------------------|
| 1.004 | 2 | 0 3 3 | 100.20 |
| .993 | 1 | 1 3 3 | 101.77 |
| .976 | 2 | 1 5 2 | 104.30 |
| .961 | 1 | 2 3 3 | 106.56 |
| .954 | 1 | 5 4 1 | 107.65 |
| .948 | 2 | 1 6 1 | 108.61 |
| .945 | 1 | 2 5 2 | 109.14 |
| .940 | 1 | 4 1 3 | 110.08 |
| .934 | 2 | 4 5 1 | 111.04 |
| .933 | 1 | 6 0 2 | 111.22 |
| .933 | 1 | 5 3 2 | 111.33 |
| .931 | 1 | 6 3 1 | 111.58 |
| .922 | 1 | 6 1 2 | 113.27 |
| .921 | 1 | 2 6 1 | 113.59 |
| .884 | 1 | 2 4 3 | 121.15 |
| .874 | 2 | 7 2 1 | 123.55 |
| .874 | 1 | 5 0 3 | 123.58 |
| .872 | 3 | 0 0 4 | 124.16 |
| .865 | 2 | 5 1 3 | 125.89 |
| .855 | 2 | 1 1 4 | 128.44 |
| .854 | 1 | 4 6 0 | 128.79 |
| .847 | 4 | 3 4 3 | 130.71 |
| .845 | 1 | 6 3 2 | 131.35 |
| .837 | 1 | 2 6 2 | 133.86 |
| .835 | 4 | 2 1 4 | 134.64 |
| .830 | 2 | 0 7 1 | 136.35 |
| .827 | 1 | 1 5 3 | 137.30 |
| .824 | 1 | 7 1 2 | 138.24 |
| .811 | 3 | 2 2 4 | 143.34 |
| .808 | 2 | 2 5 3 | 144.68 |
| .804 | 1 | 3 1 4 | 146.89 |
| .801 | 2 | 5 3 3 | 148.40 |
| .797 | 2 | 3 7 0 | 150.33 |
| .794 | 1 | 6 1 3 | 152.02 |
| .793 | 1 | 1 3 4 | 152.52 |
| .792 | 2 | 6 4 2 | 153.24 |

Copper aluminum, Cu₉Al₄

Structure

Cubic, P43m (215), Z=4. The structure was determined by Bradley and Jones [1933]. It was refined first by Westman [1965] and later by Heidenstam, Johannson, and Westman [1968]. This is the same phase of the copper-aluminum system that was called δ -CuAl (or Cu₉Al₄) by Bradley and Jones [1933] and by Weibke [1934]; it was later called γ -Cu₉Al₄ by Westman [1965] because its structure is very similar to that of γ -brass.

Lattice parameters

$a = 8.7027(5) \text{ \AA}$ (published value: $8.7023(5) \text{ \AA}$) [Heidenstam et al., 1968]

Density

(calculated) 6.850 g/cm^3

Thermal parameters

Isotropic [Heidenstam et al., 1968]

Atomic positions

The parameter values used were those in table 5 [Heidenstam et al., 1968], with half the "octahedral" Cu atoms in positions 6f and the other half in positions 6g [Westman, 1965].

Scattering factors

Cu⁰, Al⁰ [Cromer and Waber, 1965]: all factors were corrected for dispersion [Cromer, 1965].

Scale factor

(integrated intensities) 63.01×10^4

Additional patterns

1. PDF card 2-1254 [Weibke, 1934]

References

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- Weibke, F. (1934). Z. anorg.u.allgem. Chem. **220**, 293.
- Westman, S. (1965). Acta Chem. Scand. **19**, 1411.

| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|----------|----------------------------|---------------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{ }^\circ)$ | $\lambda = 1.54056 \text{ \AA}$ |
| 8.699 | 3 | 1 0 0 | 10.16 | |
| 6.154 | 1 | 1 1 0 | 14.38 | |
| 3.8903 | 4 | 2 1 0 | 22.84 | |
| 3.5533 | 8 | 2 1 1 | 25.04 | |
| 2.9006 | 8 | 3 0 0 + | 30.80 | |
| 2.5116 | 2 | 2 2 2 | 35.72 | |
| 2.3259 | 3 | 3 2 1 | 38.68 | |
| 2.0509 | 100 | 3 3 0 + | 44.12 | |
| 1.8990 | 1 | 4 2 1 | 47.86 | |
| 1.8553 | 4 | 3 3 2 | 49.06 | |
| 1.7762 | 4 | 4 2 2 | 51.40 | |
| 1.7066 | 1 | 5 1 0 + | 53.66 | |
| 1.6749 | 1 | 5 1 1 + | 54.76 | |
| 1.5150 | 1 | 5 2 2 | 61.12 | |
| 1.4503 | 8 | 6 0 0 + | 64.16 | |
| 1.4116 | 2 | 6 1 1 + | 66.14 | |
| 1.2832 | 2 | 6 3 1 | 73.78 | |
| 1.2562 | 3 | 4 4 4 | 75.64 | |
| 1.2306 | 2 | 5 5 0 + | 77.50 | |
| 1.1844 | 12 | 6 3 3 + | 81.14 | |
| 1.1053 | 1 | 7 3 2 | 88.36 | |
| 1.0712 | 5 | 7 4 1 | 91.96 | |
| 1.0553 | 1 | 8 2 0 + | 93.76 | |
| 1.0256 | 2 | 6 6 0 + | 97.36 | |
| .9173 | 2 | 9 3 0 + | 114.22 | |
| .8791 | 3 | 8 5 3 + | 122.38 | |
| .8617 | 1 | 10 1 1 + | 126.74 | |
| .8374 | 1 | 10 2 2 + | 133.80 | |
| .8151 | 4 | 7 7 4 + | 141.82 | |
| .7944 | 2 | 10 4 2 | 151.66 | |

Copper aluminum, Cu₉Al₄ - continued

| Calculated Pattern (Integrated) | | | |
|---------------------------------|-----|--------|------------------------|
| d (Å) | I | hkl | 2θ(°) λ = 1.54056 Å |
| 8.703 | 3 | 1 0 0 | 10.16 |
| 6.154 | 1 | 1 1 0 | 14.38 |
| 3.8920 | 5 | 2 1 0 | 22.83 |
| 3.5529 | 10 | 2 1 1 | 25.04 |
| 2.9009 | 6 | 3 0 0 | 30.80 |
| 2.9009 | 4 | 2 2 1 | 30.80 |
| 2.5123 | 4 | 2 2 2 | 35.71 |
| 2.3259 | 4 | 3 2 1 | 38.68 |
| 2.1107 | 1 | 3 2 2 | 42.81 |
| 2.0513 | 100 | 3 3 0 | 44.11 |
| 2.0513 | 53 | 4 1 1 | 44.11 |
| 1.9460 | 1 | 4 2 0 | 46.64 |
| 1.8991 | 1 | 4 2 1 | 47.86 |
| 1.8554 | 6 | 3 3 2 | 49.06 |
| 1.7764 | 6 | 4 2 2 | 51.39 |
| 1.7067 | 1 | 4 3 1 | 53.66 |
| 1.7067 | 1 | 5 1 0 | 53.66 |
| 1.6748 | 1 | 5 1 1 | 54.76 |
| 1.6748 | 1 | 3 3 3 | 54.76 |
| 1.6161 | 1 | 4 3 2 | 56.93 |
| 1.5150 | 1 | 5 2 2 | 61.12 |
| 1.4505 | 8 | 6 0 0 | 64.15 |
| 1.4505 | 6 | 4 4 2 | 64.15 |
| 1.4118 | 2 | 0 1 1 | 66.13 |
| 1.4118 | 1 | 5 3 2 | 66.13 |
| 1.2831 | 3 | 6 3 1 | 73.78 |
| 1.2561 | 6 | 4 4 4 | 75.65 |
| 1.2307 | 3 | 5 5 0 | 77.49 |
| 1.2307 | 1 | 5 4 3 | 77.49 |
| 1.2069 | 1 | 0 4 0 | 79.32 |
| 1.1843 | 11 | 7 2 1 | 81.15 |
| 1.1843 | 1 | 5 5 2 | 81.15 |
| 1.1843 | 14 | 6 3 3 | 81.15 |
| 1.1629 | 1 | 6 4 2 | 82.96 |
| 1.1052 | 2 | 7 3 2 | 88.36 |
| 1.0712 | 12 | 7 4 1 | 91.95 |
| 1.0554 | 1 | 8 2 0 | 93.75 |
| 1.0554 | 1 | 6 4 4 | 93.75 |
| 1.0256 | 1 | 8 2 2 | 97.36 |
| 1.0256 | 4 | 6 6 0 | 97.36 |
| .9983 | 2 | 6 6 2 | 101.00 |
| .9854 | 2 | 7 5 2 | 102.83 |
| .9174 | 3 | 9 3 0 | 114.21 |
| .9174 | 2 | 7 5 4 | 114.21 |
| .8791 | 2 | 9 4 1 | 122.38 |
| .8791 | 0 | 8 5 3 | 122.38 |
| .8617 | 1 | 7 7 2 | 126.74 |
| .8617 | 3 | 10 1 1 | 126.74 |
| .8534 | 2 | 8 6 2 | 129.01 |
| .8453 | 1 | 9 4 3 | 131.36 |

| d (Å) | I | hkl | 2θ(°) λ = 1.54056 Å |
|-------|----|--------|------------------------|
| .8374 | 3 | 10 2 2 | 133.80 |
| .8374 | 1 | 6 6 6 | 133.80 |
| .8298 | 1 | 9 5 2 | 136.34 |
| .8151 | 2 | 8 7 1 | 141.83 |
| .8151 | 12 | 7 7 4 | 141.83 |
| .8151 | 2 | 8 5 5 | 141.83 |
| .8046 | 1 | 8 7 2 | 146.43 |
| .8046 | 1 | 10 4 1 | 146.43 |
| .8012 | 1 | 10 3 3 | 148.09 |
| .8012 | 2 | 9 6 1 | 148.09 |
| .7944 | 10 | 10 4 2 | 151.66 |
| .7879 | 2 | 9 5 4 | 155.72 |
| .7879 | 2 | 11 1 0 | 155.72 |

Copper cadmium, Cu₅Cd₈

Structure

Cubic, I₄3m (217), Z=4. The structure was determined by Bradley and Gregory [1931] and refined by Heidenstam et al., [1968].

Lattice parameters

a=9.5892(3) Å (published value: 9.5888(3) Å) [Heidenstam et al., 1968]

Density
(calculated) 9.166 g/cm³

Thermal parameters

Isotropic [Heidenstam et al., 1968]

Atomic positions

Cu(1) in 8c, Cu(2) in 8c. The 12(Cu,Cd) in 12e and 24(Cu,Cd) in 24g are in random arrangement in each site, in the ratio of 1 Cu to 8 Cd.

Scattering factors

Cu⁰, Cd⁰ [Cromer and Waber, 1965]. All factors were corrected for dispersion [Cromer, 1965].

Scale factor

(integrated intensities) 159.5 × 10⁴

Reference

- Bradley, A.J. and Gregory, C.H. (1931). Phil. Mag. 12, 143.
 Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
 Cromer, D.T. (1965). Acta Cryst. 18, 17.
 v. Heidenstam, O., Johansson, A., and Westman, S. (1968). Acta Chem. Scand. 22, 653.

| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|-----|---|------------------------|
| d (Å) | I | hkl | | 2θ(°) λ = 1.54056 Å |
| 3.9140 | 1 | 2 | 1 | 22.70 |
| 3.0315 | 9 | 3 | 1 | 29.44 |
| 2.7676 | 9 | 2 | 2 | 32.32 |
| 2.5630 | 14 | 3 | 2 | 34.98 |
| 2.3976 | 1 | 4 | 0 | 37.48 |
| 2.2597 | 100 | 4 | 1 | 39.86 |
| 2.0448 | 12 | 3 | 3 | 44.26 |
| 1.9577 | 7 | 4 | 2 | 46.34 |
| 1.8805 | 3 | 5 | 1 | 48.36 |
| 1.6445 | 1 | 5 | 3 | 55.86 |
| 1.5984 | 3 | 4 | 4 | 57.62 |
| 1.5556 | 2 | 5 | 3 | 59.36 |
| 1.5163 | 1 | 6 | 2 | 61.06 |
| 1.4797 | 2 | 5 | 4 | 62.74 |
| 1.4455 | 1 | 6 | 2 | 64.40 |
| 1.4139 | 4 | 6 | 3 | 66.02 |
| 1.3839 | 4 | 4 | 4 | 67.64 |
| 1.3562 | 4 | 5 | 5 | 69.22 |
| 1.3048 | 10 | 7 | 2 | 72.36 |
| 1.2814 | 1 | 6 | 4 | 73.90 |
| 1.2177 | 2 | 7 | 3 | 78.48 |
| 1.1803 | 2 | 7 | 4 | 81.48 |
| 1.1629 | 1 | 8 | 2 | 82.96 |
| 1.1301 | 1 | 6 | 6 | 85.94 |
| 1.1000 | 1 | 6 | 6 | 88.90 |
| 1.0857 | 2 | 7 | 5 | 90.38 |
| 1.0107 | 1 | 8 | 5 | 99.30 |
| .9687 | 2 | 8 | 5 | 105.34 |
| .9228 | 1 | 10 | 2 | 113.18 |
| .8981 | 1 | 7 | 7 | 118.12 |
| .8543 | 3 | 10 | 5 | 128.76 |
| .8284 | 1 | 11 | 3 | 136.82 |

Copper cadmium, Cu₅Cd₈ - continued

| Calculated Pattern (Integrated) | | | |
|---------------------------------|-----|--------|------------------------|
| d (Å) | I | hkl | 2θ(°) λ = 1.54056 Å |
| 3.9148 | 1 | 2 1 1 | 22.70 |
| 3.0324 | 15 | 3 1 0 | 29.43 |
| 2.7682 | 15 | 2 2 2 | 32.31 |
| 2.5628 | 24 | 3 2 1 | 34.98 |
| 2.3973 | 2 | 4 0 0 | 37.48 |
| 2.2602 | 88 | 3 3 0 | 39.85 |
| 2.2602 | 100 | 4 1 1 | 39.85 |
| 2.0444 | 23 | 3 3 2 | 44.27 |
| 1.9574 | 14 | 4 2 2 | 46.35 |
| 1.8806 | 4 | 5 1 0 | 48.36 |
| 1.8806 | 2 | 4 3 1 | 48.36 |
| 1.7507 | 1 | 5 2 1 | 52.20 |
| 1.6445 | 2 | 5 3 0 | 55.86 |
| 1.6445 | 1 | 4 3 3 | 55.86 |
| 1.5982 | 2 | 6 0 0 | 57.63 |
| 1.5982 | 5 | 4 4 2 | 57.63 |
| 1.5556 | 1 | 6 1 1 | 59.36 |
| 1.5556 | 3 | 5 3 2 | 59.36 |
| 1.5162 | 2 | 6 2 0 | 61.07 |
| 1.4797 | 5 | 5 4 1 | 62.74 |
| 1.4456 | 3 | 6 2 2 | 64.39 |
| 1.4138 | 9 | 6 3 1 | 66.02 |
| 1.3841 | 9 | 4 4 4 | 67.63 |
| 1.3561 | 1 | 5 4 3 | 69.22 |
| 1.3561 | 7 | 5 5 0 | 69.22 |
| 1.3049 | 18 | 7 2 1 | 72.35 |
| 1.3049 | 1 | 5 5 2 | 72.35 |
| 1.3049 | 7 | 5 3 3 | 72.35 |
| 1.2814 | 2 | 5 4 2 | 73.90 |
| 1.2178 | 3 | 5 5 1 | 78.47 |
| 1.2178 | 3 | 7 3 2 | 78.47 |
| 1.1987 | 1 | 8 0 0 | 79.98 |
| 1.1804 | 5 | 7 4 1 | 81.47 |
| 1.1629 | 2 | 8 2 0 | 82.97 |
| 1.1629 | 2 | 6 4 4 | 82.97 |
| 1.1461 | 2 | 6 5 3 | 84.45 |
| 1.1301 | 2 | 6 6 0 | 85.94 |
| 1.1301 | 2 | 8 2 2 | 85.94 |
| 1.1000 | 3 | 6 6 2 | 88.90 |
| 1.0858 | 5 | 7 5 2 | 90.38 |
| 1.0590 | 1 | 8 3 3 | 93.34 |
| 1.0340 | 1 | 9 2 1 | 96.31 |
| 1.0108 | 1 | 7 5 4 | 99.29 |
| 1.0108 | 1 | 8 5 1 | 99.29 |
| .9891 | 1 | 9 3 2 | 102.30 |
| .9787 | 1 | 8 4 4 | 103.82 |
| .9687 | 2 | 9 4 1 | 105.35 |
| .9687 | 5 | 8 5 3 | 105.35 |
| .9495 | 1 | 10 1 1 | 108.44 |
| .9314 | 2 | 9 5 0 | 111.59 |

| d (Å) | I | hkl | 2θ(°) λ = 1.54056 Å |
|-------|---|--------|------------------------|
| .9227 | 4 | 10 2 2 | 113.19 |
| .9227 | 1 | 6 6 6 | 113.19 |
| .8981 | 2 | 8 7 1 | 118.11 |
| .8981 | 3 | 7 7 4 | 118.11 |
| .8981 | 1 | 8 5 5 | 118.11 |
| .8682 | 2 | 9 5 4 | 125.06 |
| .8543 | 2 | 11 2 1 | 128.76 |
| .8543 | 5 | 9 6 3 | 128.76 |
| .8543 | 6 | 10 5 1 | 128.76 |
| .8476 | 2 | 8 8 0 | 130.68 |
| .8410 | 1 | 9 7 0 | 132.66 |
| .8346 | 1 | 10 4 4 | 134.71 |
| .8284 | 2 | 11 3 2 | 136.83 |
| .8284 | 1 | 7 7 6 | 136.83 |
| .8223 | 1 | 10 6 0 | 139.03 |
| .8223 | 1 | 8 6 6 | 139.03 |
| .8163 | 1 | 8 7 5 | 141.34 |
| .8163 | 1 | 11 4 1 | 141.34 |
| .8047 | 2 | 9 6 5 | 146.36 |
| .7991 | 2 | 8 8 4 | 149.13 |
| .7936 | 1 | 9 7 4 | 152.15 |
| .7936 | 1 | 11 5 0 | 152.15 |
| .7936 | 1 | 12 1 1 | 152.15 |
| .7936 | 1 | 11 4 3 | 152.15 |
| .7829 | 2 | 11 5 2 | 159.35 |

Copper hydrogen phosphite hydrate, CuHPO₃·2H₂O

Structure

Orthorhombic, P2₁2₁2₁ (19), z=4. The structure was determined by Handlovic [1969].

Lattice parameters

a=6.71, b=9.00, c=7.40 Å [ibid.]

Density (calculated) 2.67 g/cm³

Thermal parameters

Isotropic [Handlovic]

Scattering factors

Cu⁰, O⁰, P⁰ [International Tables, 1962]

Scale factor

(integrated intensities) 4.158 × 10⁴

Reference

Handlovic, M. (1969). Acta Cryst. B25, 227
International Tables for X-ray Crystallography III
(1962). 202, 210.

| <i>d</i> (Å) | <i>I</i> | Calculated Pattern (<i>Peak heights</i>) | | | <i>2θ(°)</i> $\lambda = 1.54056 \text{ Å}$ |
|--------------|----------|--|---|-----|---|
| | | <i>hkl</i> | | | |
| 5.38 | 22 | 1 | 1 | 0 | 16.46 |
| 4.97 | 100 | 1 | 0 | 1 | 17.84 |
| 4.50 | 3 | 0 | 2 | 0 | 19.72 |
| 4.35 | 10 | 1 | 1 | 1 | 20.40 |
| 3.84 | 10 | 0 | 2 | 1 | 23.12 |
| 3.74 | 63 | 1 | 2 | 0 | 23.80 |
| 3.70 | 10 | 0 | 0 | 2 | 24.04 |
| 3.422 | 21 | 0 | 1 | 2 | 26.02 |
| 3.336 | 13 | 1 | 2 | 1 | 26.70 |
| 3.241 | 7 | 1 | 0 | 2 | 27.50 |
| 2.893 | 10 | 2 | 1 | 1 + | 30.88 |
| 2.857 | 2 | 0 | 2 | 2 | 31.28 |
| 2.779 | 7 | 0 | 3 | 1 | 32.18 |
| 2.690 | 9 | 2 | 2 | 0 | 33.28 |
| 2.629 | 8 | 1 | 2 | 2 | 34.08 |
| 2.569 | 4 | 1 | 3 | 1 | 34.90 |
| 2.528 | 38 | 2 | 2 | 1 | 35.48 |
| 2.485 | 2 | 2 | 0 | 2 | 36.12 |
| 2.395 | 5 | 2 | 1 | 2 | 37.52 |
| 2.379 | 1 | 0 | 1 | 3 | 37.78 |
| 2.331 | 1 | 0 | 3 | 2 | 38.60 |
| 2.316 | 9 | 1 | 0 | 3 | 38.86 |
| 2.250 | 4 | 0 | 4 | 0 | 40.04 |
| 2.242 | 5 | 1 | 1 | 3 | 40.18 |
| 2.237 | 4 | 2 | 3 | 0 | 40.28 |
| 2.170 | 3 | 3 | 1 | 0 | 41.58 |
| 2.163 | 7 | 0 | 2 | 3 | 41.72 |
| 2.152 | 3 | 0 | 4 | 1 | 41.94 |
| 2.141 | 4 | 3 | 0 | 1 | 42.18 |
| 2.134 | 5 | 1 | 4 | 0 | 42.32 |
| 2.059 | 4 | 1 | 2 | 3 | 43.94 |
| 2.050 | 7 | 1 | 4 | 1 | 44.14 |
| 2.003 | 0 | 3 | 2 | 0 | 45.24 |
| 1.940 | 2 | 2 | 1 | 3 | 46.78 |
| 1.933 | 2 | 3 | 2 | 1 | 46.96 |
| 1.914 | 3 | 3 | 0 | 2 + | 47.46 |
| 1.905 | 2 | 0 | 3 | 3 | 47.70 |
| 1.869 | 1 | 2 | 4 | 0 | 48.68 |
| 1.848 | 5 | 1 | 4 | 2 + | 49.26 |
| 1.833 | 4 | 1 | 3 | 3 | 49.70 |
| 1.818 | 3 | 2 | 2 | 3 | 50.14 |
| 1.812 | 5 | 2 | 4 | 1 + | 50.32 |
| 1.793 | 1 | 3 | 3 | 0 | 50.88 |
| 1.783 | 1 | 1 | 0 | 4 | 51.18 |
| 1.762 | 4 | 3 | 2 | 2 | 51.86 |
| 1.750 | 4 | 1 | 1 | 4 | 52.24 |
| 1.745 | 2 | 3 | 3 | 1 | 52.40 |
| 1.711 | 1 | 0 | 2 | 4 | 53.52 |
| 1.693 | 2 | 1 | 5 | 1 | 54.14 |
| 1.678 | 5 | 4 | 0 | 0 | 54.66 |

Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ – continued

| d (Å) | I | hkl | 2θ (°) | $\lambda = 1.54056$ Å |
|---------|-----|---------|---------------|-----------------------|
| | | | ° | |
| 1.668 | 6 | 2 4 2 | 55.00 | |
| 1.663 | 4 | 0 4 3 | 55.18 | |
| 1.658 | 6 | 1 2 4 + | 55.38 | |
| 1.649 | 1 | 4 1 0 | 55.68 | |
| 1.630 | 1 | 3 1 3 | 56.42 | |
| 1.620 | 3 | 2 0 4 | 56.78 | |
| 1.614 | 3 | 1 4 3 | 57.02 | |
| 1.594 | 2 | 2 1 4 | 57.78 | |
| 1.586 | 1 | 3 4 0 | 58.10 | |
| 1.573 | 2 | 1 5 2 + | 58.62 | |
| 1.555 | 1 | 3 2 3 | 59.40 | |
| 1.551 | 3 | 3 4 1 | 59.56 | |
| 1.537 | 1 | 4 2 1 | 60.14 | |
| 1.528 | 1 | 4 0 2 | 60.56 | |
| 1.506 | 1 | 4 1 2 | 61.52 | |
| 1.490 | 2 | 2 4 3 | 62.28 | |
| 1.458 | 2 | 3 4 2 + | 63.78 | |
| 1.454 | 2 | 0 5 3 | 63.98 | |
| 1.450 | 2 | 3 3 3 | 64.16 | |
| 1.447 | 2 | 4 2 2 | 64.34 | |
| 1.436 | 3 | 1 6 1 + | 64.88 | |
| 1.425 | 3 | 2 3 4 + | 65.42 | |
| 1.408 | 1 | 3 1 4 | 66.34 | |
| 1.398 | 1 | 1 4 4 | 66.88 | |
| 1.390 | 2 | 0 6 2 | 67.30 | |
| 1.369 | 2 | 2 6 0 | 68.46 | |
| 1.361 | 1 | 4 3 2 + | 68.92 | |
| 1.359 | 2 | 3 2 4 | 69.06 | |
| 1.345 | 1 | 4 4 0 | 69.88 | |
| 1.339 | 1 | 2 1 5 | 70.24 | |
| 1.334 | 1 | 2 5 3 + | 70.52 | |
| 1.325 | 2 | 4 2 3 | 71.06 | |
| 1.322 | 1 | 4 4 1 | 71.26 | |
| 1.320 | 2 | 5 0 1 | 71.38 | |
| 1.315 | 1 | 2 4 4 | 71.74 | |
| 1.306 | 1 | 5 1 1 | 72.26 | |
| 1.302 | 1 | 1 3 5 | 72.54 | |
| 1.297 | 2 | 2 2 5 | 72.88 | |
| 1.286 | 1 | 5 2 0 | 73.60 | |
| 1.284 | 2 | 2 6 2 | 73.70 | |
| 1.281 | 1 | 0 6 3 | 73.90 | |
| 1.267 | 2 | 5 2 1 + | 74.88 | |
| 1.259 | 2 | 1 6 3 + | 75.44 | |
| 1.228 | 1 | 3 6 1 | 77.66 | |
| 1.216 | 1 | 1 4 5 | 78.62 | |
| 1.141 | 1 | 3 3 5 + | 84.88 | |
| 1.112 | 1 | 0 8 1 + | 87.68 | |
| 1.074 | 1 | 0 2 1 | 91.68 | |
| 1.070 | 1 | 4 6 2 | 92.04 | |
| 1.063 | 1 | 1 8 2 | 92.90 | |
| 1.006 | 1 | 1 5 6 | 99.96 | |

| Calculated Pattern (Integrated) | | | | |
|---------------------------------|-----|-------|---------------|-----------------------|
| d (Å) | I | hkl | 2θ (°) | $\lambda = 1.54056$ Å |
| 5.38 | 21 | 1 1 0 | 16.46 | |
| 4.97 | 100 | 1 0 1 | 17.83 | |
| 4.50 | 3 | 0 2 0 | 19.71 | |
| 4.35 | 10 | 1 1 1 | 20.39 | |
| 3.84 | 17 | 0 2 1 | 23.11 | |
| 3.74 | 70 | 1 2 0 | 23.79 | |
| 3.70 | 9 | 0 0 2 | 24.03 | |
| 3.422 | 23 | 0 1 2 | 26.02 | |
| 3.355 | 1 | 2 0 0 | 26.55 | |
| 3.336 | 14 | 1 2 1 | 26.70 | |
| 3.240 | 8 | 1 0 2 | 27.51 | |
| 3.056 | 3 | 2 0 1 | 29.20 | |
| 3.049 | 10 | 1 1 2 | 29.27 | |
| 2.893 | 11 | 2 1 1 | 30.88 | |
| 2.858 | 2 | 0 2 2 | 31.27 | |
| 2.780 | 9 | 0 3 1 | 32.17 | |
| 2.690 | 11 | 2 2 0 | 33.28 | |
| 2.629 | 10 | 1 2 2 | 34.07 | |
| 2.568 | 4 | 1 3 1 | 34.90 | |
| 2.528 | 45 | 2 2 1 | 35.48 | |
| 2.485 | 3 | 2 0 2 | 36.11 | |
| 2.396 | 6 | 2 1 2 | 37.51 | |
| 2.379 | 1 | 0 1 3 | 37.78 | |
| 2.330 | 1 | 0 3 2 | 38.60 | |
| 2.315 | 11 | 1 0 3 | 38.87 | |
| 2.250 | 5 | 0 4 0 | 40.04 | |
| 2.242 | 5 | 1 1 3 | 40.19 | |
| 2.236 | 2 | 2 3 0 | 40.30 | |
| 2.171 | 3 | 3 1 0 | 41.57 | |
| 2.163 | 8 | 0 2 3 | 41.72 | |
| 2.153 | 3 | 0 4 1 | 41.93 | |
| 2.141 | 5 | 3 0 1 | 42.17 | |
| 2.133 | 5 | 1 4 0 | 42.33 | |
| 2.059 | 5 | 1 2 3 | 43.94 | |
| 2.050 | 9 | 1 4 1 | 44.15 | |
| 2.003 | 8 | 3 2 0 | 45.24 | |
| 1.941 | 3 | 2 1 3 | 46.77 | |
| 1.933 | 2 | 3 2 1 | 46.96 | |
| 1.914 | 2 | 3 0 2 | 47.46 | |
| 1.914 | 1 | 2 3 2 | 47.46 | |
| 1.905 | 2 | 0 3 3 | 47.69 | |
| 1.869 | 2 | 2 4 0 | 48.69 | |
| 1.850 | 3 | 0 0 4 | 49.21 | |
| 1.848 | 5 | 1 4 2 | 49.27 | |
| 1.833 | 5 | 1 3 3 | 49.70 | |
| 1.818 | 3 | 2 2 3 | 50.14 | |
| 1.812 | 1 | 0 1 4 | 50.31 | |
| 1.812 | 5 | 2 4 1 | 50.32 | |
| 1.793 | 1 | 3 3 0 | 50.88 | |
| 1.783 | 1 | 1 0 4 | 51.18 | |

Copper hydrogen phosphite hydrate, CuHPO₃·2H₂O – continued

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2θ(°) $\lambda = 1.54056 \text{ Å}$ | <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2θ(°) $\lambda = 1.54056 \text{ Å}$ |
|--------------|----------|------------|--|--------------|----------|------------|--|
| 1.761 | 0 | 3 2 2 | 51.87 | 1.297 | 4 | 2 2 5 | 72.89 |
| 1.749 | 5 | 1 1 4 | 52.25 | 1.286 | 1 | 5 2 0 | 73.59 |
| 1.743 | 1 | 3 3 1 | 52.46 | 1.284 | 2 | 2 6 2 | 73.71 |
| 1.711 | 2 | 0 2 4 | 53.51 | 1.282 | 1 | 0 6 3 | 73.89 |
| 1.692 | 2 | 1 5 1 | 54.15 | 1.267 | 1 | 5 2 1 | 74.88 |
| 1.677 | 8 | 4 0 0 | 54.67 | 1.267 | 1 | 1 5 4 | 74.89 |
| 1.668 | 8 | 2 4 2 | 55.01 | 1.259 | 1 | 4 3 3 | 75.44 |
| 1.662 | 1 | 0 4 3 | 55.21 | 1.259 | 1 | 1 6 3 | 75.45 |
| 1.658 | 6 | 1 2 4 | 55.37 | 1.249 | 1 | 5 1 2 | 76.13 |
| 1.657 | 2 | 3 0 3 | 55.41 | 1.228 | 2 | 5 6 1 | 77.66 |
| 1.649 | 1 | 4 1 0 | 55.69 | 1.216 | 1 | 1 4 5 | 78.61 |
| 1.630 | 2 | 3 1 3 | 56.42 | 1.204 | 1 | 3 4 4 | 79.53 |
| 1.620 | 4 | 2 0 4 | 56.78 | 1.179 | 1 | 5 0 3 | 81.60 |
| 1.614 | 3 | 1 4 3 | 57.03 | 1.169 | 1 | 5 1 3 | 82.45 |
| 1.594 | 2 | 2 1 4 | 57.78 | 1.143 | 1 | 0 5 5 | 84.72 |
| 1.586 | 2 | 3 4 0 | 58.10 | 1.142 | 1 | 2 7 2 | 84.83 |
| 1.575 | 1 | 0 3 4 | 58.57 | 1.141 | 1 | 3 3 5 | 84.88 |
| 1.573 | 3 | 1 5 2 | 58.62 | 1.141 | 1 | 0 3 6 | 84.95 |
| 1.555 | 1 | 3 2 3 | 59.39 | 1.124 | 1 | 1 7 3 | 86.52 |
| 1.551 | 4 | 3 4 1 | 59.55 | 1.112 | 2 | 0 8 1 | 87.67 |
| 1.538 | 2 | 4 2 1 | 60.13 | 1.112 | 1 | 3 6 3 | 87.69 |
| 1.528 | 1 | 4 0 2 | 60.55 | 1.074 | 1 | 0 2 1 | 91.67 |
| 1.506 | 2 | 4 1 2 | 61.51 | 1.072 | 1 | 3 1 6 | 91.83 |
| 1.490 | 4 | 2 4 3 | 62.28 | 1.070 | 1 | 4 6 2 | 92.05 |
| 1.458 | 2 | 3 4 2 | 63.79 | 1.063 | 2 | 1 8 2 | 92.90 |
| 1.458 | 1 | 2 5 2 | 63.79 | 1.018 | 1 | 4 6 3 | 98.29 |
| 1.454 | 1 | 0 5 3 | 63.98 | 1.006 | 1 | 1 5 6 | 99.95 |
| 1.450 | 2 | 3 3 3 | 64.16 | 1.002 | 2 | 2 1 7 | 100.48 |
| 1.447 | 1 | 4 2 2 | 64.34 | .991 | 1 | 5 6 1 | 102.00 |
| 1.436 | 1 | 4 3 1 | 64.86 | .986 | 1 | 1 3 7 | 102.71 |
| 1.436 | 4 | 1 6 1 | 64.88 | .979 | 1 | 2 8 3 | 103.77 |
| 1.427 | 1 | 1 1 5 | 65.34 | .970 | 1 | 3 8 2 | 105.16 |
| 1.425 | 3 | 2 3 4 | 65.42 | .967 | 1 | 6 4 2 | 105.66 |
| 1.408 | 2 | 3 1 4 | 66.33 | .945 | 1 | 4 5 5 | 109.25 |
| 1.398 | 2 | 1 4 4 | 66.89 | .944 | 1 | 5 3 5 | 109.42 |
| 1.390 | 2 | 0 6 2 | 67.30 | | | | |
| 1.369 | 3 | 2 6 0 | 68.46 | | | | |
| 1.361 | 1 | 4 3 2 | 68.91 | | | | |
| 1.361 | 1 | 1 6 2 | 68.93 | | | | |
| 1.359 | 3 | 3 2 4 | 69.06 | | | | |
| 1.345 | 1 | 4 4 0 | 69.89 | | | | |
| 1.339 | 2 | 2 1 5 | 70.23 | | | | |
| 1.334 | 1 | 3 4 3 | 70.53 | | | | |
| 1.334 | 1 | 2 5 3 | 70.53 | | | | |
| 1.326 | 3 | 4 2 3 | 71.05 | | | | |
| 1.323 | 1 | 4 4 1 | 71.20 | | | | |
| 1.320 | 2 | 5 0 1 | 71.37 | | | | |
| 1.315 | 2 | 2 4 4 | 71.73 | | | | |
| 1.306 | 1 | 5 1 1 | 72.26 | | | | |
| 1.302 | 2 | 1 3 5 | 72.54 | | | | |

L-Cysteine, $\text{HSCH}_2\text{-CH}(\text{NH}_2)\text{COOH}$

Structure

Monoclinic, $P2_1(4)$, $Z=4$. The structure was determined by Harding and Long [1968].

Lattice parameters

$a=11.51(1)$, $b=5.240(5)$, $c=9.517(10)\text{\AA}$, $\beta=109.13^\circ$
[ibid.]

Density

(calculated) 1.484 g/cm^3

Thermal parameters

| | | | |
|------------|------------|----------------|------|
| Isotropic: | carbon (1) | 1.26 | |
| | " (11) | 1.26 | |
| sulfur (1) | B=3.81 | nitrogen (1) | 1.26 |
| sulfur (2) | 4.99 | " (11) | 1.74 |
| carbon (3) | 2.37 | oxygen (1) | 1.58 |
| " (13) | 2.21 | " (11) | 1.74 |
| " (2) | 1.58 | " (2) | 2.45 |
| " (12) | 1.42 | " (12) | 2.45 |
| | | hydrogen (all) | 1.42 |

Scattering factors

C^0 , H^0 , N^0 , $O^{-\frac{1}{2}}$, S^0 . The sulfur factors were corrected for the real part of the dispersion. [International Tables, 1962].

Scale factor

(integrated intensities) 0.5947×10^4

Additional patterns

1. PDF card 13-722 [Eli Lilly Co., Indianapolis, Indiana.]

Reference

Harding, M.M. and Long, H.A. (1968). Acta Cryst. B24, 1096.
International Tables for X-ray Crystallography III (1962), 202, 214.

| Calculated Pattern (Peak heights) | | | |
|-----------------------------------|-----|----------|--|
| $d (\text{\AA})$ | I | hkl | $2\theta (^\circ)$ $\lambda = 1.54056 \text{\AA}$ |
| 10.88 | 42 | 1 0 0 | 8.12 |
| 8.98 | 4 | 0 0 1 | 9.84 |
| 8.40 | 1 | -1 0 1 | 10.52 |
| 6.02 | 3 | 1 0 1 | 14.70 |
| 5.52 | 2 | -2 0 1 | 16.04 |
| 5.43 | 11 | 2 0 0 | 16.30 |
| 4.72 | 86 | 1 1 0 + | 18.78 |
| 4.53 | 100 | 0 1 1 | 19.60 |
| 4.49 | 92 | 0 0 2 | 19.74 |
| 4.45 | 34 | -1 1 1 | 19.94 |
| 4.21 | 14 | -2 0 2 | 21.10 |
| 3.96 | 14 | 1 1 1 | 22.46 |
| 3.82 | 4 | -3 0 1 | 23.24 |
| 3.802 | 15 | -2 1 1 | 23.38 |
| 3.773 | 29 | 2 1 0 | 23.56 |
| 3.745 | 41 | 1 0 2 | 23.74 |
| 3.625 | 44 | 3 0 0 | 24.54 |
| 3.515 | 54 | -1 1 2 | 25.32 |
| 3.422 | 34 | -3 0 2 | 26.02 |
| 3.411 | 51 | 0 1 2 | 26.10 |
| 3.281 | 20 | -2 1 2 | 27.16 |
| 3.227 | 58 | 2 1 1 | 27.62 |
| 3.166 | 4 | -1 0 3 | 28.16 |
| 3.087 | 15 | -2 0 3 + | 28.90 |
| 3.046 | 3 | 1 1 2 | 29.30 |
| 3.035 | 3 | 3 0 1 | 29.40 |
| 2.996 | 7 | 0 0 3 | 29.80 |
| 2.980 | 53 | 3 1 0 | 29.96 |
| 2.866 | 4 | -3 1 2 | 31.18 |
| 2.805 | 1 | -3 0 3 | 31.88 |
| 2.761 | 19 | -4 0 2 | 32.40 |
| 2.719 | 50 | 4 0 0 | 32.92 |
| 2.712 | 41 | -1 1 3 | 33.00 |
| 2.673 | 3 | 1 0 3 | 33.50 |
| 2.660 | 25 | -2 1 3 | 33.66 |
| 2.626 | 7 | 3 1 1 | 34.12 |
| 2.620 | 11 | 0 2 0 | 34.20 |
| 2.612 | 11 | 2 1 2 | 34.30 |
| 2.605 | 6 | 0 1 3 | 34.40 |
| 2.547 | 9 | 1 2 0 | 35.20 |
| 2.516 | 4 | 0 2 1 | 35.66 |
| 2.502 | 3 | -1 2 1 | 35.86 |
| 2.473 | 7 | -3 1 3 | 36.30 |
| 2.456 | 14 | 3 0 2 | 36.56 |
| 2.443 | 8 | -4 1 2 | 36.76 |
| 2.412 | 2 | 4 1 0 | 37.24 |
| 2.403 | 2 | 1 2 1 | 37.40 |
| 2.394 | 2 | 4 0 1 | 37.54 |
| 2.382 | 17 | 1 1 3 | 37.74 |
| 2.370 | 9 | -2 0 4 | 37.94 |

L-Cysteine, $\text{HSCH}_2\text{-CH}(\text{NH}_2)\text{-COOH}$ – continued

| d (Å) | I | hkl | $2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$ | d (Å) | I | hkl | $2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|----------|--|---------|-----|----------|--|
| 2.360 | 6 | 2 2 0 + | 38.10 | 1.673 | 3 | 5 2 0 | 54.82 |
| 2.293 | 2 | -1 2 2 + | 39.26 | 1.663 | 4 | 2 3 0 + | 55.18 |
| 2.273 | 6 | -3 0 4 | 39.62 | 1.628 | 2 | 0 3 2 | 56.48 |
| 2.248 | 11 | 0 0 4 | 40.08 | 1.613 | 3 | -2 3 2 + | 57.04 |
| 2.221 | 15 | -4 1 3 + | 40.58 | 1.607 | 3 | 1 1 5 + | 57.30 |
| 2.208 | 2 | 2 2 1 | 40.84 | 1.599 | 3 | 3 1 4 | 57.58 |
| 2.177 | 4 | 4 1 1 | 41.44 | 1.594 | 3 | 6 1 1 | 57.78 |
| 2.161 | 5 | -3 2 1 + | 41.76 | 1.583 | 2 | 1 3 2 | 58.24 |
| 2.155 | 3 | -1 1 4 | 41.88 | 1.573 | 1 | 3 3 0 + | 58.62 |
| 2.146 | 4 | 1 2 2 | 42.06 | 1.569 | 2 | -7 1 2 | 58.82 |
| 2.121 | 5 | -5 0 3 + | 42.58 | 1.557 | 1 | -6 0 5 | 59.32 |
| 2.104 | 2 | -4 0 4 | 42.96 | 1.553 | 2 | 7 0 0 + | 59.46 |
| 2.100 | 2 | -5 1 1 | 43.04 | 1.543 | 2 | -4 0 6 | 59.88 |
| 2.085 | 6 | -3 1 4 + | 43.36 | 1.541 | 2 | -5 2 4 + | 59.98 |
| 2.081 | 8 | -3 2 2 | 43.46 | 1.529 | 1 | -1 3 3 | 60.48 |
| 2.066 | 1 | 0 1 4 | 43.78 | 1.525 | 1 | -3 2 5 | 60.68 |
| 2.048 | 1 | 4 0 2 | 44.18 | 1.507 | 2 | 4 0 4 | 61.50 |
| 2.019 | 1 | -1 2 3 | 44.86 | 1.496 | 1 | 2 1 5 | 61.96 |
| 2.009 | 1 | 3 0 3 | 45.10 | 1.493 | 2 | -4 3 1 | 62.14 |
| 1.998 | 1 | -2 2 3 | 45.36 | 1.490 | 3 | 6 2 0 + | 62.24 |
| 1.983 | 4 | 3 2 1 | 45.72 | 1.483 | 2 | 0 2 5 | 62.60 |
| 1.977 | 13 | 2 2 2 | 45.86 | 1.475 | 1 | 5 1 3 + | 62.96 |
| 1.972 | 9 | 5 0 1 + | 45.98 | 1.458 | 1 | 6 1 2 | 63.80 |
| 1.967 | 3 | -5 1 3 | 46.12 | 1.453 | 2 | 5 2 2 | 64.02 |
| 1.952 | 1 | -4 1 4 | 46.48 | 1.419 | 1 | 1 2 5 | 65.76 |
| 1.937 | 1 | -4 2 1 | 46.86 | 1.406 | 1 | -2 3 4 | 66.44 |
| 1.926 | 1 | -1 1 4 | 47.16 | 1.384 | 1 | 3 1 5 | 67.64 |
| 1.915 | 2 | -3 2 3 | 47.44 | 1.380 | 2 | -7 2 1 + | 67.88 |
| 1.907 | 7 | 4 1 2 | 47.64 | 1.376 | 1 | -8 1 3 | 68.08 |
| 1.901 | 7 | -4 2 2 | 47.82 | 1.373 | 1 | -7 2 3 | 68.26 |
| 1.886 | 1 | 4 2 0 | 48.20 | 1.339 | 1 | -6 2 5 + | 70.26 |
| 1.875 | 2 | 3 1 3 + | 48.50 | 1.313 | 2 | 6 2 2 | 71.84 |
| 1.871 | 3 | 1 2 3 + | 48.62 | 1.310 | 2 | -2 1 7 | 72.02 |
| 1.845 | 2 | 5 1 1 | 49.36 | 1.297 | 1 | 7 1 2 | 72.84 |
| 1.841 | 3 | -6 0 3 | 49.48 | 1.294 | 1 | -1 4 1 | 73.04 |
| 1.798 | 4 | 0 0 5 + | 50.72 | 1.287 | 1 | -2 3 5 | 73.54 |
| 1.794 | 4 | -4 0 5 | 50.86 | 1.275 | 1 | -9 0 3 | 74.34 |
| 1.791 | 5 | -5 1 4 + | 50.94 | 1.271 | 1 | -8 1 5 | 74.58 |
| 1.787 | 3 | -6 1 1 | 51.06 | 1.261 | 1 | -8 2 2 | 75.32 |
| 1.764 | 7 | -3 1 5 + | 51.78 | 1.252 | 1 | -4 3 5 | 75.96 |
| 1.760 | 5 | -2 2 4 | 51.92 | | | | |
| 1.753 | 3 | -1 2 4 | 52.12 | | | | |
| 1.749 | 2 | 4 0 3 | 52.26 | | | | |
| 1.737 | 5 | -6 1 3 | 52.66 | | | | |
| 1.725 | 1 | 1 3 0 + | 53.06 | | | | |
| 1.715 | 4 | 0 3 1 + | 53.38 | | | | |
| 1.711 | 3 | -6 0 4 | 53.50 | | | | |
| 1.706 | 3 | 0 2 4 | 53.68 | | | | |
| 1.701 | 2 | 0 1 5 | 53.84 | | | | |
| 1.678 | 1 | 1 3 1 + | 54.66 | | | | |

L-Cysteine, $\text{HSCH}_2\text{-CH}(\text{NH}_2)\text{-COOH}$ – continued

| Calculated Pattern (Integrated) | | | | d (\AA) | I | hkl | $2\theta (\text{ }^\circ)$ $\lambda = 1.54056 \text{ \AA}$ | $2\theta (\text{ }^\circ)$ $\lambda = 1.54056 \text{ \AA}$ |
|---------------------------------|-----|--------|--|----------------------|-------|-----------|---|---|
| 10.87 | 38 | 1 0 0 | | 8.12 | 21 | 1 1 3 | 37.74 | |
| 8.99 | 8 | 0 0 1 | | 9.83 | 10 | -2 0 4 | 37.94 | |
| 8.41 | 1 | -1 0 1 | | 10.50 | 3 | 2 2 0 | 38.10 | |
| 6.03 | 3 | 1 0 1 | | 14.69 | 3 | -1 0 4 | 38.10 | |
| 5.52 | 2 | -2 0 1 | | 16.04 | 1 | -1 2 2 | 39.26 | |
| 5.44 | 11 | 2 0 0 | | 16.29 | 2.293 | 1 -5 0 1 | 39.27 | |
| 4.74 | 42 | -1 0 2 | | 18.71 | 2.293 | 2 -3 0 4 | 39.62 | |
| 4.72 | 71 | 1 1 0 | | 18.78 | 2.248 | 13 0 0 4 | 40.08 | |
| 4.53 | 100 | 0 1 1 | | 19.59 | 2.224 | 7 -2 2 2 | 40.53 | |
| 4.50 | 89 | 0 0 2 | | 19.73 | 2.224 | 1 3 1 2 | 40.53 | |
| 4.45 | 32 | -1 1 1 | | 19.94 | 2.222 | 15 -4 1 3 | 40.57 | |
| 4.21 | 15 | -2 0 2 | | 21.10 | 2.207 | 2 2 2 1 | 40.85 | |
| 3.95 | 15 | 1 1 1 | | 22.46 | 2.177 | 5 4 1 1 | 41.43 | |
| 3.82 | 3 | -3 0 1 | | 23.24 | 2.161 | 5 -3 2 1 | 41.76 | |
| 3.801 | 15 | -2 1 1 | | 23.38 | 2.159 | 2 -2 1 4 | 41.80 | |
| 3.773 | 29 | 2 1 0 | | 23.56 | 2.152 | 1 -1 1 4 | 41.95 | |
| 3.744 | 45 | 1 0 2 | | 23.75 | 2.147 | 4 1 2 2 | 42.06 | |
| 3.625 | 49 | 3 0 0 | | 24.54 | 2.123 | 3 2 1 3 | 42.54 | |
| 3.515 | 61 | -1 1 2 | | 25.32 | 2.104 | 5 -5 0 3 | 42.58 | |
| 3.423 | 31 | -3 0 2 | | 26.01 | 2.100 | 2 -5 1 1 | 42.96 | |
| 3.412 | 44 | 0 1 2 | | 26.09 | 2.085 | 6 -3 1 4 | 43.36 | |
| 3.281 | 23 | -2 1 2 | | 27.16 | 2.084 | 1 -5 1 2 | 43.39 | |
| 3.227 | 67 | 2 1 1 | | 27.62 | 2.080 | 6 -3 2 2 | 43.46 | |
| 3.168 | 5 | -1 0 3 | | 28.15 | 2.066 | 2 0 1 4 | 43.79 | |
| 3.089 | 9 | -3 1 1 | | 28.88 | 2.048 | 1 4 0 2 | 44.19 | |
| 3.087 | 10 | -2 0 3 | | 28.90 | 2.019 | 1 -1 2 3 | 44.86 | |
| 3.046 | 3 | 1 1 2 | | 29.29 | 2.009 | 1 3 0 3 | 45.09 | |
| 3.035 | 2 | 3 0 1 | | 29.41 | 1.998 | 1 -2 2 3 | 45.36 | |
| 2.997 | 5 | 0 0 3 | | 29.78 | 1.983 | 4 3 2 1 | 45.71 | |
| 2.981 | 67 | 3 1 0 | | 29.95 | 1.977 | 17 2 2 2 | 45.86 | |
| 2.866 | 5 | -3 1 2 | | 31.19 | 1.973 | 1 0 2 3 | 45.97 | |
| 2.805 | 1 | -3 0 3 | | 31.88 | 1.971 | 2 5 0 1 | 46.00 | |
| 2.761 | 23 | -4 0 2 | | 32.40 | 1.966 | 1 -5 1 3 | 46.12 | |
| 2.719 | 59 | 4 0 0 | | 32.92 | 1.952 | 1 -4 1 4 | 46.48 | |
| 2.671 | 17 | -1 1 3 | | 33.02 | 1.937 | 1 -4 2 1 | 46.87 | |
| 2.674 | 2 | 1 0 3 | | 33.49 | 1.926 | 1 1 1 4 | 47.15 | |
| 2.660 | 32 | -2 1 3 | | 33.67 | 1.915 | 2 -3 2 3 | 47.44 | |
| 2.626 | 6 | 3 1 1 | | 34.11 | 1.908 | 9 4 1 2 | 47.63 | |
| 2.620 | 9 | 0 2 0 | | 34.20 | 1.901 | 8 -4 2 2 | 47.82 | |
| 2.612 | 9 | 2 1 2 | | 34.30 | 1.887 | 1 4 2 0 | 48.20 | |
| 2.602 | 3 | 0 1 3 | | 34.44 | 1.876 | 1 -1 0 5 | 48.49 | |
| 2.547 | 11 | 1 2 0 | | 35.21 | 1.872 | 1 2 0 4 | 48.60 | |
| 2.515 | 5 | 0 2 1 | | 35.66 | 1.871 | 3 1 2 3 | 48.61 | |
| 2.502 | 4 | -1 2 1 | | 35.87 | 1.845 | 2 5 1 1 | 49.35 | |
| 2.473 | 8 | -3 1 3 | | 36.30 | 1.841 | 3 -6 0 3 | 49.47 | |
| 2.456 | 17 | 3 0 2 | | 36.56 | 1.798 | 5 0 0 5 | 50.72 | |
| 2.443 | 9 | -4 1 2 | | 36.76 | 1.796 | 2 -6 1 2 | 50.78 | |
| 2.413 | 2 | 4 1 0 | | 37.23 | 1.795 | 1 -4 0 5 | 50.83 | |
| 2.403 | 1 | 1 2 1 | | 37.40 | | | | |
| 2.394 | 4 | 4 0 1 | | 37.54 | | | | |

L-Cysteine, $\text{HSCH}_2\text{-CH}(\text{NH}_2)\text{-COOH}$ – continued

| d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ |
|----------------------|-----|--------|--|
| 1.792 | 2 | 3 2 2 | 50.92 |
| 1.791 | 2 | -5 1 4 | 50.94 |
| 1.791 | 2 | -4 2 3 | 50.96 |
| 1.789 | 1 | -2 1 5 | 51.01 |
| 1.787 | 1 | -6 1 1 | 51.06 |
| 1.766 | 2 | -1 1 5 | 51.72 |
| 1.764 | 9 | -3 1 5 | 51.77 |
| 1.763 | 2 | 2 1 4 | 51.82 |
| 1.757 | 1 | -2 2 4 | 51.99 |
| 1.753 | 3 | -1 2 4 | 52.12 |
| 1.749 | 1 | 4 0 3 | 52.27 |
| 1.737 | 7 | -6 1 3 | 52.66 |
| 1.725 | 1 | -5 2 1 | 53.03 |
| 1.725 | 1 | 1 3 0 | 53.06 |
| 1.717 | 1 | -3 2 4 | 53.31 |
| 1.716 | 2 | -5 2 2 | 53.34 |
| 1.715 | 4 | 0 3 1 | 53.39 |
| 1.713 | 1 | 6 1 0 | 53.45 |
| 1.711 | 1 | -6 0 4 | 53.50 |
| 1.706 | 4 | 0 2 4 | 53.68 |
| 1.701 | 1 | 0 1 5 | 53.85 |
| 1.680 | 1 | 3 0 4 | 54.59 |
| 1.678 | 1 | 1 3 1 | 54.66 |
| 1.673 | 4 | 5 2 0 | 54.81 |
| 1.665 | 1 | -2 3 1 | 55.10 |
| 1.663 | 6 | 2 3 0 | 55.19 |
| 1.626 | 2 | 0 3 2 | 56.47 |
| 1.614 | 1 | 4 2 2 | 57.03 |
| 1.613 | 3 | -2 3 2 | 57.04 |
| 1.612 | 1 | -7 0 3 | 57.10 |
| 1.607 | 2 | 2 3 1 | 57.30 |
| 1.606 | 2 | 1 1 5 | 57.31 |
| 1.599 | 4 | 3 1 4 | 57.58 |
| 1.594 | 4 | 6 1 1 | 57.78 |
| 1.583 | 3 | 1 3 2 | 58.24 |
| 1.575 | 1 | 5 2 1 | 58.55 |
| 1.574 | 1 | 3 3 0 | 58.62 |
| 1.569 | 3 | -7 1 2 | 58.82 |
| 1.557 | 2 | -6 0 5 | 59.31 |
| 1.555 | 1 | -1 0 6 | 59.38 |
| 1.553 | 2 | 7 0 0 | 59.45 |
| 1.544 | 2 | -4 0 6 | 59.87 |
| 1.541 | 2 | -5 2 4 | 59.97 |
| 1.539 | 1 | -6 2 1 | 60.07 |
| 1.530 | 2 | -1 3 3 | 60.48 |
| 1.524 | 1 | -3 2 5 | 60.71 |
| 1.507 | 2 | 4 0 4 | 61.49 |
| 1.497 | 1 | 2 1 5 | 61.96 |
| 1.493 | 2 | -4 3 1 | 62.12 |
| 1.491 | 2 | 6 2 0 | 62.23 |

| d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ |
|----------------------|-----|--------|--|
| 1.489 | 2 | 7 1 0 | 62.29 |
| 1.483 | 2 | 0 2 5 | 62.60 |
| 1.476 | 1 | -4 3 2 | 62.91 |
| 1.475 | 1 | 5 1 3 | 62.97 |
| 1.462 | 1 | 1 3 3 | 63.57 |
| 1.457 | 2 | 6 1 2 | 63.81 |
| 1.453 | 1 | 5 2 2 | 64.02 |
| 1.419 | 1 | 1 2 5 | 65.77 |
| 1.406 | 1 | -2 3 4 | 66.44 |
| 1.384 | 1 | 3 1 5 | 67.65 |
| 1.380 | 1 | -7 1 5 | 67.88 |
| 1.379 | 1 | -7 2 1 | 67.89 |
| 1.376 | 1 | -8 1 3 | 68.08 |
| 1.373 | 1 | -7 2 3 | 68.26 |
| 1.348 | 1 | -5 3 3 | 69.67 |
| 1.344 | 1 | -4 0 7 | 69.94 |
| 1.339 | 1 | 7 0 2 | 70.23 |
| 1.338 | 2 | -6 2 5 | 70.27 |
| 1.330 | 1 | -4 2 6 | 70.79 |
| 1.313 | 2 | 6 2 2 | 71.84 |
| 1.310 | 2 | -2 1 7 | 72.01 |
| 1.297 | 1 | 7 1 2 | 72.84 |
| 1.294 | 1 | -1 4 1 | 73.04 |
| 1.287 | 1 | -2 3 5 | 73.53 |
| 1.275 | 1 | -9 0 3 | 74.35 |
| 1.271 | 1 | -8 1 5 | 74.59 |
| 1.261 | 1 | -8 2 2 | 75.32 |
| 1.252 | 1 | -4 3 5 | 75.96 |

Iron fluoride hydrate, $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$

Structure

Hexagonal, $\bar{R}\bar{3}m$ (166), $Z=3$. The structure was determined by Penfold and Taylor [1960].

Lattice parameters

$a=9.50(1)$, $c=4.82(1)$ Å [ibid.]

Density (calculated) 2.19 g/cm³

Thermal parameters

Isotropic [ibid.]

Atomic positions

In a disordered atomic arrangement, the 6 fluoride atoms and 12 water molecules were found to occupy one set of 36-fold positions, each site containing on the average ($\frac{1}{6}\text{F}^-$ and $\frac{1}{3}\text{O}^0$). The hydrogen positions were not determined [ibid.].

Polymorphism

Two kinds of white crystals precipitated together: the form "A", described here, and a form "B" which appeared to have a very similar structure with the c doubled [ibid.]

Scattering factors

Fe^{2+} [Thomas and Umeda, 1957]
 $(\frac{1}{6}\text{F}^- + \frac{1}{3}\text{O}^0)$ [Berghuis et al., 1955].

Scale factor

(integrated intensities) 3.406×10^4

Additional patterns

1. PDF card 22-626 [Ostrovskaya and Amirova, 1969]

| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|-------|---------------|-----------------------|
| d (Å) | I | hkl | 2θ (°) | $\lambda = 1.54056$ Å |
| 4.75 | 100 | 1 1 0 | 18.66 | |
| 4.16 | 57 | 1 0 1 | 21.36 | |
| 3.13 | 5 | 0 2 1 | 28.50 | |
| 2.74 | 1 | 3 0 0 | 32.62 | |
| 2.61 | 35 | 2 1 1 | 34.30 | |
| 2.374 | 1 | 2 2 0 | 37.86 | |
| 2.080 | 5 | 2 0 2 | 43.48 | |
| 2.062 | 1 | 1 3 1 | 43.86 | |
| 1.905 | 12 | 1 2 2 | 47.70 | |
| 1.892 | 9 | 4 0 1 | 48.06 | |
| 1.795 | 5 | 4 1 0 | 50.82 | |
| 1.758 | 5 | 3 2 1 | 51.98 | |
| 1.657 | 8 | 3 1 2 | 55.40 | |
| 1.583 | 2 | 3 3 0 | 58.22 | |
| 1.564 | 1 | 0 4 2 | 59.00 | |
| 1.557 | 1 | 0 5 1 | 59.30 | |
| 1.522 | 2 | 1 1 3 | 60.82 | |
| 1.486 | 2 | 2 3 2 | 62.44 | |
| 1.480 | 2 | 2 4 1 | 62.74 | |
| 1.413 | 1 | 5 1 1 | 66.08 | |
| 1.386 | 2 | 0 3 3 | 67.52 | |
| 1.371 | 1 | 6 0 0 | 68.36 | |
| 1.331 | 1 | 2 2 3 | 70.74 | |
| 1.317 | 2 | 5 2 0 | 71.56 | |
| 1.214 | 1 | 1 6 1 | 78.76 | |
| 1.197 | 1 | 1 4 3 | 80.08 | |
| 1.192 | 1 | 1 0 4 | 80.48 | |
| 1.142 | 1 | 3 5 1 | 84.84 | |

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Iron fluoride hydrate, $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ – continued

| Calculated Pattern (<i>Integrated</i>) | | | | |
|--|-----|-------|--|--|
| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056$ Å | |
| 4.75 | 100 | 1 1 0 | 18.67 | |
| 4.16 | 60 | 1 0 1 | 21.35 | |
| 3.13 | 5 | 0 2 1 | 28.50 | |
| 2.74 | 1 | 3 0 0 | 32.03 | |
| 2.61 | 42 | 2 1 1 | 34.29 | |
| 2.375 | 1 | 2 2 0 | 37.85 | |
| 2.079 | 5 | 2 0 2 | 43.48 | |
| 2.062 | 1 | 1 3 1 | 43.86 | |
| 1.905 | 15 | 1 2 2 | 47.70 | |
| 1.892 | 11 | 4 0 1 | 48.05 | |
| 1.795 | 7 | 4 1 0 | 50.81 | |
| 1.758 | 7 | 3 2 1 | 51.99 | |
| 1.657 | 11 | 3 1 2 | 55.40 | |
| 1.583 | 2 | 3 3 0 | 58.22 | |
| 1.565 | 2 | 0 4 2 | 58.99 | |
| 1.557 | 1 | 0 5 1 | 59.29 | |
| 1.522 | 3 | 1 1 3 | 60.81 | |
| 1.486 | 3 | 2 3 2 | 62.45 | |
| 1.480 | 3 | 2 4 1 | 62.74 | |
| 1.413 | 2 | 5 1 1 | 66.08 | |
| 1.386 | 3 | 0 3 3 | 67.51 | |
| 1.371 | 2 | 6 0 0 | 68.35 | |
| 1.331 | 2 | 2 2 3 | 70.74 | |
| 1.317 | 3 | 5 2 0 | 71.56 | |
| 1.307 | 1 | 4 2 2 | 72.25 | |
| 1.302 | 1 | 4 3 1 | 72.53 | |
| 1.214 | 2 | 1 6 1 | 78.75 | |
| 1.197 | 2 | 1 4 3 | 80.09 | |
| 1.192 | 1 | 1 0 4 | 80.49 | |
| 1.142 | 2 | 3 5 1 | 84.84 | |
| 1.128 | 1 | 3 3 3 | 86.16 | |
| 1.019 | 1 | 5 2 3 | 98.25 | |
| .965 | 1 | 4 5 2 | 105.89 | |
| .944 | 1 | 8 1 1 | 109.32 | |
| .934 | 1 | 5 1 4 | 111.14 | |
| .926 | 1 | 4 6 1 | 112.55 | |
| .871 | 1 | 6 3 3 | 124.35 | |
| .812 | 1 | 9 1 2 | 143.10 | |
| .807 | 1 | 1 5 5 | 145.13 | |
| .799 | 1 | 9 2 1 | 148.96 | |
| .795 | 1 | 0 9 3 | 151.61 | |
| .785 | 1 | 3 4 5 | 157.76 | |
| .784 | 1 | 2 8 3 | 158.80 | |

Lithium hydroxide hydrate, LiOH·H₂O

Structure

Monoclinic, I2/m (12), Z=4. Pepinsky [1939] determined the structure and published his data in terms of the C2/m cell with $a=7.37\text{ kX}$, $b=8.26\text{ kX}$, $c=3.19\text{ kX}$, and $\beta=110^\circ 18'$. Rabaud and Gay [1955] did further work, and Alcock [1971] refined their data to determine all the hydrogen positions.

Lattice parameters

$a=6.95$, $b=8.28$, $c=3.20\text{ \AA}$, $\beta=95.23^\circ$.

Density

(calculated) 1.53 g/cm^3

Thermal parameters

Isotropic: hydrogen(1):B=12.3;hydrogen(2):B=14.0 [Alcock,1971]; lithium: B=3.82; oxygen(1):B=2.87 oxygen(2): B=4.67.

Atomic positions

Alcock [1971].

Scattering factors

Li^+ , O^0 [International Tables, 1962]
 H^0 [McWeeny, 1951]

Scale factor

(integrated intensities) 0.1301×10^4

Additional patterns

1. PDF card 1-1062 [Dow Chemical Co., Midland, Michigan].

Reference

- Alcock, N.W. (1971). Acta Cryst. B27, 1682.
- International Tables for X-ray Crystallography III 1962, pg. 202.
- McWeeny, R. (1951). Acta Cryst. 4, 513.
- Pepinsky, R. (1937). Z. Krist. 102A, 119.
- Rabaud, H. and Gay, R. (1957). Bull. Soc. Franç. Minéral Crist. 80, 166.

| Calculated Pattern (Peak heights) | | | | | $2\theta (\text{ }^\circ)$ $\lambda = 1.54056 \text{ \AA}$ |
|-----------------------------------|-----|--------|---|--|---|
| $d (\text{\AA})$ | I | hkl | | | |
| 4.14 | 2 | C 2 0 | | | 21.44 |
| 3.47 | 3 | -2 0 0 | | | 25.68 |
| 2.97 | 66 | 0 1 1 | | | 30.02 |
| 2.80 | 24 | 1 0 1 | | | 31.94 |
| 2.66 | 100 | -2 2 0 | | | 33.70 |
| 2.56 | 11 | -1 3 0 | | | 34.96 |
| 2.43 | 45 | -1 2 1 | | | 36.96 |
| 2.225 | 6 | -3 1 0 | | | 40.50 |
| 2.167 | 3 | 2 1 1 | | | 41.64 |
| 2.086 | 1 | C 3 1 | | | 43.34 |
| 2.070 | 6 | 0 4 0 | | | 43.70 |
| 1.958 | 8 | -3 0 1 | | | 46.34 |
| 1.836 | 9 | -2 3 1 | | | 49.60 |
| 1.777 | 3 | -2 4 0 | | | 51.38 |
| 1.742 | 13 | 2 3 1 | | | 52.48 |
| 1.733 | 6 | -4 0 0 | | | 52.78 |
| 1.664 | 3 | 1 4 1 | | | 55.14 |
| 1.646 | 1 | 3 2 1 | | | 55.80 |
| 1.611 | 1 | -1 5 0 | | | 57.14 |
| 1.593 | 2 | C 0 2 | | | 57.82 |
| 1.557 | 2 | -1 1 2 | | | 59.32 |
| 1.500 | 2 | -2 0 2 | | | 61.78 |
| 1.497 | 2 | 1 1 2 | | | 61.92 |
| 1.470 | 3 | C 5 1 | | | 63.22 |
| 1.445 | 2 | 4 1 1 | | | 64.44 |
| 1.422 | 3 | -3 4 1 | | | 65.58 |
| 1.380 | 1 | C 6 0 | | | 67.86 |
| 1.374 | 2 | -1 3 2 | + | | 68.18 |
| 1.367 | 1 | -5 1 0 | | | 68.58 |
| 1.353 | 1 | -3 1 2 | | | 69.40 |
| 1.346 | 1 | -3 5 0 | | | 69.82 |
| 1.326 | 1 | 2 2 2 | | | 71.02 |
| 1.254 | 1 | -5 2 1 | + | | 75.80 |
| 1.179 | 1 | -4 2 2 | | | 81.56 |

Lithium hydroxide hydrate, LiOH·H₂O – continued

| Calculated Pattern (<i>Integrated</i>) | | | | |
|--|----------|------------|--|--|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2θ (°) $\lambda = 1.54056 \text{ Å}$ | |
| 4.14 | 2 | 0 2 0 | 21.45 | |
| 3.47 | 3 | -2 0 0 | 25.68 | |
| 2.97 | 64 | 0 1 1 | 30.02 | |
| 2.80 | 24 | 1 0 1 | 31.94 | |
| 2.66 | 100 | -2 2 0 | 33.70 | |
| 2.56 | 11 | -1 3 0 | 34.96 | |
| 2.43 | 46 | -1 2 1 | 36.96 | |
| 2.225 | 6 | -3 1 0 | 40.50 | |
| 2.167 | 4 | 2 1 1 | 41.64 | |
| 2.086 | 1 | 0 3 1 | 43.33 | |
| 2.070 | 7 | 0 4 0 | 43.69 | |
| 1.957 | 10 | -3 0 1 | 46.35 | |
| 1.837 | 11 | -2 3 1 | 49.59 | |
| 1.777 | 3 | -2 4 0 | 51.37 | |
| 1.742 | 16 | 2 3 1 | 52.49 | |
| 1.733 | 7 | -4 0 0 | 52.79 | |
| 1.664 | 4 | 1 4 1 | 55.13 | |
| 1.646 | 1 | 3 2 1 | 55.80 | |
| 1.611 | 1 | -1 5 0 | 57.14 | |
| 1.593 | 3 | 0 0 2 | 57.82 | |
| 1.557 | 2 | -1 1 2 | 59.32 | |
| 1.501 | 2 | -2 0 2 | 61.77 | |
| 1.498 | 2 | 1 1 2 | 61.91 | |
| 1.469 | 4 | 0 5 1 | 63.23 | |
| 1.445 | 3 | 4 1 1 | 64.45 | |
| 1.422 | 4 | -3 4 1 | 65.59 | |
| 1.380 | 1 | 0 6 0 | 67.86 | |
| 1.374 | 2 | -1 3 2 | 68.18 | |
| 1.374 | 1 | -4 3 1 | 68.20 | |
| 1.367 | 1 | -5 1 0 | 68.58 | |
| 1.353 | 1 | -3 1 2 | 69.40 | |
| 1.346 | 2 | -3 5 0 | 69.82 | |
| 1.326 | 2 | 2 2 2 | 71.02 | |
| 1.254 | 1 | -5 2 1 | 75.79 | |
| 1.254 | 1 | -1 6 1 | 75.81 | |
| 1.239 | 1 | -5 3 0 | 76.90 | |
| 1.179 | 1 | -4 2 2 | 81.57 | |
| 1.121 | 1 | 1 5 2 | 86.82 | |
| 1.098 | 1 | 4 5 1 | 89.09 | |

Magnesium chloride (chloromagnesite), MgCl_2

Structure

Hexagonal, $R\bar{3}m$ (166), $Z=3$, isostructural with CdCl_2 . The structure was determined by Pauling [1929].

Lattice parameters

$a=3.632(4)$, $c=17.795(16)\text{\AA}$ [Ferrari et al., 1963]

Density

(calculated) 3.540 g/cm^3

Thermal parameters

Isotropic, overall $B=2.0$

Scattering factors

Mg^{2+} , Cl^- [International Tables, 1962]

Scale factor

(integrated intensities) 1.022×10^4

Reference

- Ferrari, A., Braibanti, A., and Bigliardi, G. (1963).
Acta Cryst. **16**, 846.
Hanawalt, J.D., Rinn, H.W., and Frevel, L.K. (1938).
Ind. Eng. Chem. Anal. Ed. **10**, 457.
International Tables for X-ray Crystallography III
(1962), pg. 202.
Pauling, L. (1929). Proc. Nat'l. Acad. Sci. USA **15**,
709.

| Calculated Pattern (Integrated) | | | | |
|---------------------------------|-----|--------|--|--|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{ }^\circ)$ $\lambda = 1.54056 \text{\AA}$ | |
| 5.93 | 19 | 0 0 3 | 14.92 | |
| 3.097 | 12 | 1 0 1 | 28.80 | |
| 2.966 | 13 | 0 0 6 | 30.10 | |
| 2.966 | 40 | 0 1 2 | 30.11 | |
| 2.568 | 100 | 1 0 4 | 34.90 | |
| 2.357 | 5 | 0 1 5 | 38.15 | |
| 1.977 | 1 | 0 0 9 | 45.85 | |
| 1.977 | 3 | 1 0 7 | 45.86 | |
| 1.816 | 20 | 0 1 8 | 50.19 | |
| 1.816 | 26 | 1 1 0 | 50.20 | |
| 1.736 | 3 | 1 1 3 | 52.67 | |
| 1.567 | 1 | 0 2 1 | 58.90 | |
| 1.549 | 2 | 1 0 10 | 59.64 | |
| 1.549 | 5 | 1 1 6 | 59.65 | |
| 1.549 | 2 | 2 0 2 | 59.65 | |
| 1.483 | 4 | 0 0 12 | 62.58 | |
| 1.483 | 11 | 0 2 4 | 62.60 | |
| 1.439 | 1 | 0 1 11 | 64.74 | |
| 1.439 | 1 | 2 0 5 | 64.75 | |
| 1.338 | 1 | 1 1 9 | 70.32 | |
| 1.284 | 6 | 2 0 8 | 73.71 | |
| 1.179 | 1 | 0 1 14 | 81.63 | |
| 1.178 | 1 | 0 2 10 | 81.63 | |
| 1.178 | 2 | 1 2 2 | 81.64 | |
| 1.149 | 7 | 1 1 12 | 84.23 | |
| 1.149 | 7 | 2 1 4 | 84.24 | |
| 1.049 | 2 | 1 0 16 | 94.54 | |
| 1.049 | 5 | 1 2 8 | 94.55 | |
| 1.048 | 2 | 3 0 0 | 94.56 | |
| .989 | 1 | 2 1 10 | 102.38 | |
| .908 | 2 | 0 2 16 | 116.04 | |
| .908 | 2 | 2 2 0 | 116.06 | |
| .868 | 1 | 1 1 18 | 125.02 | |
| .868 | 1 | 1 2 14 | 125.03 | |
| .868 | 1 | 2 2 6 | 125.04 | |
| .868 | 1 | 3 1 2 | 125.05 | |
| .856 | 2 | 0 1 20 | 128.22 | |
| .856 | 2 | 3 0 12 | 128.25 | |
| .856 | 2 | 0 3 12 | 128.25 | |
| .856 | 3 | 1 3 4 | 128.26 | |
| .812 | 4 | 2 1 16 | 143.02 | |
| .812 | 4 | 3 1 8 | 143.04 | |
| .783 | 1 | 1 0 22 | 158.98 | |
| .783 | 2 | 1 3 10 | 159.06 | |
| .783 | 1 | 0 4 2 | 159.08 | |

Additional patterns

1. PDF 3-0854 [Hanwalt et al., 1938]

Manganese oxide (partridgeite), alpha Mn₂O₃ (revised)

Structure

Orthorhombic, Pcab (61), Z=16. The structure was determined by Norrestam [1967] and confirmed by Geller [1971]. The structure had previously been reported as a cubic, C-type sesquioxide [Pauling and Shappell, 1930; Swanson et al., 1960].

Lattice parameters

a=9.4161(3), b=9.4237(3), c=9.4051(3) Å (published values: 9.4157(3), 9.4233(3), 9.4047(3) Å) [Geller, 1971]

Density (calculated) 5.026 g/cm³

Thermal parameters

Isotropic:

| | | | |
|--------------|---------|------------|---------|
| Manganese(1) | B=0.335 | oxygen(6) | B=0.641 |
| Manganese(2) | B=0.416 | oxygen(7) | B=0.684 |
| Manganese(3) | B=0.577 | oxygen(8) | B=0.606 |
| Manganese(4) | B=0.584 | oxygen(9) | B=0.517 |
| Manganese(5) | B=0.573 | oxygen(10) | B=0.629 |
| | | oxygen(11) | B=0.598 |

Atomic positions

Geller [1971]

Polymorphism

Above 35°C, α-Mn₂O₃ becomes cubic. (Substitution of less than one cation % Fe³⁺ for the Mn³⁺ ion makes the compound cubic, at room temperature.) [Geller, 1971]. The alpha form described here was called β-Mn₂O₃ by Morozov and Kuznetcov [1949]. A polymorph called γ-Mn₂O₃ was prepared by dehydration of Mn₂O₃·H₂O, and was somewhat unstable [Verwey and deBoer, 1936].

Scattering factors

Mn³⁺ [Cromer and Waber, 1965], corrected for dispersion [Cromer, 1965].
O²⁻ [Tokonami, 1965]

| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|---------|--------|---------------|
| d (Å) | I | hkl | 2θ (°) | λ = 1.54056 Å |
| 4.706 | 1 | 0 0 2 + | 18.84 | |
| 3.844 | 18 | 1 1 2 + | 23.12 | |
| 3.1379 | <1 | 2 1 2 + | 28.42 | |
| 2.7185 | 100 | 2 2 2 | 32.92 | |
| 2.5157 | 2 | 3 1 2 + | 35.66 | |
| 2.3540 | 11 | 0 4 0 + | 38.20 | |
| 2.2192 | <1 | 4 1 1 + | 40.62 | |
| 2.1054 | <1 | 2 4 0 + | 42.92 | |
| 2.0069 | 9 | 3 3 2 + | 45.14 | |
| 1.9210 | 1 | 2 2 4 + | 47.28 | |
| 1.8462 | 10 | 3 4 1 + | 49.32 | |
| 1.7191 | 2 | 5 1 2 + | 53.24 | |
| 1.6643 | 27 | 4 4 0 + | 55.14 | |
| 1.6143 | 2 | 3 3 4 + | 57.00 | |
| 1.5686 | <1 | 0 0 6 + | 58.82 | |
| 1.5272 | 2 | 1 1 6 + | 60.58 | |
| 1.4887 | <1 | 6 0 2 + | 62.32 | |
| 1.4524 | 4 | 5 1 4 + | 64.06 | |
| 1.4196 | 11 | 2 6 2 + | 65.72 | |
| 1.3883 | 3 | 6 1 3 + | 67.40 | |
| 1.3589 | 3 | 4 4 4 | 69.06 | |
| 1.3314 | <1 | 3 5 4 + | 70.70 | |
| 1.3052 | <1 | 4 6 0 + | 72.34 | |
| 1.2814 | 1 | 1 7 2 + | 73.90 | |
| 1.2802 | 1 | 2 1 7 + | 73.98 | |
| 1.2585 | <1 | 6 4 2 + | 75.48 | |
| 1.1956 | <1 | 5 6 1 + | 80.22 | |
| 1.1772 | 1 | 0 8 0 + | 81.74 | |
| 1.1755 | 1 | 0 0 8 | 81.88 | |
| 1.1591 | 1 | 8 1 1 + | 83.30 | |
| 1.1579 | 1 | 1 1 8 + | 83.40 | |
| 1.1419 | <1 | 8 2 0 + | 84.84 | |
| 1.1406 | <1 | 2 0 8 + | 84.96 | |
| 1.1252 | 1 | 6 5 3 + | 86.40 | |
| 1.1097 | <1 | 2 8 2 + | 87.92 | |
| 1.1087 | <1 | 2 2 8 | 88.02 | |
| 1.0945 | <1 | 1 3 8 + | 89.46 | |
| 1.0798 | 2 | 6 2 + | 91.02 | |

Scale factor

(integrated intensities) 54.67 × 10⁴

Additional patterns

1. PDF card 10-69 [Swanson et al., 1960].

References

- Geller, S. (1971). Acta Cryst. B27, 821.
 Morozov, I.S. and Kuznetcov, V.G. (1949). Izvest. Akad. Nauk. SSSR Otdel. Khim. Nauk, No. 4, 343.
 Norrestam, R. (1967). Acta Chem. Scand. 21, 19.
 Pauling, L. and Shappell, M. D. (1930). Z. Krist. 75, 128.
 Tokonami, M. (1965). Acta Cryst. 19, 486.
 Swanson, H. E., Cook, M., Isaacs, T., and Evans, E. H. (1960). Nat'l. Bur. Std. U.S. Circ. 539, No. 9, 37.
 Verwey, E.G.W., and deBoer, J.H. (1936). Rec. trav. chim. 55, 531.

Manganese oxide (partridgeite), alpha Mn₂O₃ (revised) – continued

| Calculated Pattern (<i>Integrated</i>) | | | | |
|--|----------|------------|---------------------|---------------------------------|
| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | $2\theta(^{\circ})$ | $\lambda = 1.54056 \text{ \AA}$ |
| 3.845 | 0 | 1 2 1 | 23.11 | |
| 3.844 | 5 | 2 1 1 | 23.12 | |
| 3.842 | 6 | 1 1 2 | 23.13 | |
| 2.7179 | 100 | 2 2 2 | 32.93 | |
| 2.3559 | 5 | 0 4 0 | 38.17 | |
| 2.3540 | 5 | 4 0 0 | 38.20 | |
| 2.3513 | 5 | 0 0 4 | 38.25 | |
| 2.0078 | 4 | 3 3 2 | 45.12 | |
| 2.0072 | 4 | 2 3 3 | 45.13 | |
| 2.0069 | 4 | 3 2 3 | 45.14 | |
| 1.8475 | 2 | 3 4 1 | 49.28 | |
| 1.8471 | 2 | 4 3 1 | 49.29 | |
| 1.8468 | 2 | 1 4 3 | 49.30 | |
| 1.8460 | 2 | 4 1 3 | 49.33 | |
| 1.8458 | 2 | 1 3 4 | 49.33 | |
| 1.8454 | 2 | 3 1 4 | 49.34 | |
| 1.6652 | 13 | 4 4 0 | 55.11 | |
| 1.6642 | 13 | 0 4 4 | 55.14 | |
| 1.6636 | 13 | 4 0 4 | 55.17 | |
| 1.5286 | 1 | 1 6 1 | 60.52 | |
| 1.5275 | 1 | 0 1 1 | 60.57 | |
| 1.5258 | 1 | 1 1 6 | 60.64 | |
| 1.4536 | 1 | 4 5 1 | 64.00 | |
| 1.4533 | 1 | 5 4 1 | 64.01 | |
| 1.4530 | 1 | 1 5 4 | 64.03 | |
| 1.4524 | 1 | 1 4 5 | 64.06 | |
| 1.4523 | 1 | 5 1 4 | 64.06 | |
| 1.4519 | 1 | 4 1 5 | 64.08 | |
| 1.4203 | 7 | 2 6 2 | 65.68 | |
| 1.4195 | 7 | 6 2 2 | 65.73 | |
| 1.4183 | 7 | 2 2 6 | 65.79 | |
| 1.3892 | 1 | 3 6 1 | 67.35 | |
| 1.3889 | 1 | 1 6 3 | 67.37 | |
| 1.3885 | 1 | 6 3 1 | 67.39 | |
| 1.3880 | 1 | 6 1 3 | 67.41 | |
| 1.3873 | 1 | 1 3 6 | 67.46 | |
| 1.3871 | 1 | 3 1 6 | 67.47 | |
| 1.3589 | 4 | 4 4 4 | 69.06 | |
| 1.2822 | 1 | 1 7 2 | 73.85 | |
| 1.2814 | 1 | 7 2 1 | 73.90 | |
| 1.2800 | 1 | 2 1 7 | 73.99 | |
| 1.1780 | 1 | 0 8 0 | 81.67 | |
| 1.1770 | 1 | 8 0 0 | 81.75 | |
| 1.1756 | 1 | 0 0 8 | 81.87 | |
| 1.1599 | 1 | 1 8 1 | 83.22 | |
| 1.1590 | 1 | 8 1 1 | 83.30 | |
| 1.1577 | 1 | 1 1 8 | 83.42 | |
| 1.0804 | 2 | 6 6 2 | 90.95 | |
| 1.0799 | 2 | 2 6 6 | 91.00 | |
| 1.0795 | 2 | 6 2 6 | 91.04 | |

Manganese oxide hydroxide, groutite, alpha MnOOH

Structure

Orthorhombic, Pbnm (62), $Z=4$. It is isostructural with goethite (α -FeOOH) and diaspore (α -AlOOH) [Gruner, 1947]. The groutite structure was determined by Collin and Lipscomb [1949] and refined by Glasser and Ingram [1968].

Lattice parameters

$a=4.560$, $b=10.700$, $c=2.870(\text{\AA})$ [Glasser and Ingram, 1968]

Density

(calculated) 4.171 g/cm^3

Thermal parameters

Isotropic [Glasser and Ingram, 1968]

Atomic positions

Glasser and Ingram [1968].

Polymorphism

MnOOH occurs also as two other minerals: manganese (γ form, monoclinic) and feitnechtite (β form, hexagonal).

Scattering factors

Mn^{3+} [International Tables, 1962]
 O^{2-} [Suzuki, 1960]

Scale factor

(integrated intensities) 0.7057×10^4

Additional patterns

1. PDF card 12-733 [Thompson, R.M., Univ. of British Columbia, Vancouver, British Columbia, Canada.]

Reference

Collin, R.L. and Lipscomb, W.N. (1949). Acta Cryst. 2, 104.
 Glasser, L.S.D. and Ingram, L. (1968). Acta Cryst. B24, 1233.
 International Tables for X-ray Crystallography III
 1962, 210.
 Suzuki, T. (1960). Acta Cryst. 13, 279.

| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|---------|---------------------|---------------------------------|
| $d(\text{\AA})$ | I | hkl | $2\theta(^{\circ})$ | $\lambda = 1.54056 \text{ \AA}$ |
| 5.35 | 9 | 0 2 0 | 16.56 | |
| 4.20 | 100 | 1 1 0 | 21.16 | |
| 3.471 | 10 | 1 2 0 | 25.64 | |
| 2.810 | 34 | 1 3 0 | 31.82 | |
| 2.674 | 29 | 0 4 0 | 33.48 | |
| 2.529 | 13 | 0 2 1 | 35.46 | |
| 2.429 | 4 | 1 0 1 | 36.98 | |
| 2.368 | 48 | 1 1 1 | 37.96 | |
| 2.308 | 17 | 1 4 0 | 39.00 | |
| 2.280 | 2 | 2 0 0 | 39.50 | |
| 2.230 | 2 | 2 1 0 | 40.42 | |
| 2.212 | 7 | 1 2 1 | 40.76 | |
| 2.008 | 5 | 1 3 1 | 45.12 | |
| 1.957 | 3 | 0 4 1 | 46.36 | |
| 1.937 | 4 | 1 5 0 | 46.86 | |
| 1.798 | 3 | 1 4 1 | 50.72 | |
| 1.783 | 2 | 0 6 0 | 51.18 | |
| 1.761 | 9 | 2 1 1 | 51.88 | |
| 1.735 | 6 | 2 4 0 | 52.70 | |
| 1.693 | 26 | 2 2 1 | 54.12 | |
| 1.606 | 18 | 1 5 1 | 57.34 | |
| 1.596 | 7 | 2 3 1 | 57.70 | |
| 1.560 | 3 | 2 5 0 | 59.16 | |
| 1.515 | 9 | 0 6 1 | 61.14 | |
| 1.485 | 1 | 2 4 1 | 62.50 | |
| 1.462 | 4 | 3 2 0 | 63.58 | |
| 1.449 | 4 | 1 7 0 | 64.22 | |
| 1.435 | 6 | 0 0 2 | 64.94 | |
| 1.404 | 1 | 2 6 0 | 66.52 | |
| 1.398 | 3 | 3 3 0 | 66.86 | |
| 1.358 | 3 | 1 1 2 | 69.12 | |
| 1.343 | 3 | 3 0 1 | 69.98 | |
| 1.333 | 1 | 3 1 1 | 70.62 | |
| 1.326 | 1 | 1 2 2 | 71.02 | |
| 1.303 | 1 | 3 2 1 | 72.50 | |
| 1.278 | 4 | 1 3 2 | 74.14 | |
| 1.264 | 3 | 0 4 2 | 75.06 | |
| 1.262 | 3 | 2 6 1 | 75.26 | |
| 1.257 | 2 | 3 3 1 | 75.58 | |
| 1.218 | 1 | 1 4 2 | 78.42 | |
| 1.215 | 1 | 2 0 2 | 78.72 | |
| 1.212 | 2 | 0 8 1 | 78.90 | |
| 1.200 | 3 | 3 4 1 | 79.84 | |
| 1.157 | 1 | 3 6 0 | 83.50 | |
| 1.154 | 3 | 2 8 0 + | 83.78 | |
| 1.133 | 2 | 4 1 0 | 85.62 | |
| 1.106 | 2 | 2 4 2 | 88.30 | |
| 1.078 | 1 | 3 7 0 | 91.24 | |
| 1.073 | 1 | 3 6 1 | 91.76 | |
| 1.070 | 2 | 2 8 1 + | 92.06 | |

Manganese oxide hydroxide, groutite, alpha MnOOH – continued

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|---------|--|
| 1.068 | 3 | 1 9 1 | 92.34 |
| 1.056 | 1 | 2 5 2 | 93.66 |
| 1.054 | 1 | 2 9 0 | 93.90 |
| 1.024 | 1 | 3 2 2 | 97.54 |
| 1.020 | 2 | 1 7 2 | 98.12 |
| 1.016 | 1 | 4 3 1 | 98.66 |
| 1.006 | 1 | 4 5 0 | 99.92 |
| 1.004 | 1 | 2 6 2 | 100.24 |
| 1.003 | 1 | 0 10 1 | 100.40 |
| 1.001 | 2 | 3 3 2 | 100.56 |
| .951 | 1 | 1 11 0 | 108.14 |
| .948 | 1 | 3 8 1 | 108.72 |
| .933 | 1 | 1 1 3 | 111.34 |
| .901 | 1 | 3 6 2 | 117.58 |
| .899 | 2 | 2 8 2 + | 117.90 |
| .890 | 2 | 4 1 2 | 119.98 |
| .871 | 4 | 4 7 1 + | 124.42 |
| .869 | 2 | 5 0 1 | 124.96 |
| .866 | 1 | 4 3 2 | 125.64 |
| .862 | 1 | 3 7 2 | 126.70 |
| .858 | 2 | 1 5 3 + | 127.80 |
| .856 | 1 | 2 3 3 | 128.20 |
| .854 | 1 | 2 11 1 | 128.78 |
| .852 | 1 | 0 12 1 | 129.54 |
| .850 | 1 | 2 9 2 | 130.10 |
| .843 | 1 | 0 6 3 | 132.04 |
| .827 | 1 | 5 4 1 | 137.44 |
| .824 | 1 | 4 5 2 | 138.46 |
| .823 | 1 | 3 8 2 | 138.86 |

| Calculated Pattern (Integrated) | | | |
|---------------------------------|-----|-------|--|
| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
| 5.35 | 9 | 0 2 0 | 16.56 |
| 4.19 | 100 | 1 1 0 | 21.16 |
| 3.470 | 11 | 1 2 0 | 25.65 |
| 2.809 | 40 | 1 3 0 | 31.83 |
| 2.675 | 34 | 0 4 0 | 33.47 |
| 2.529 | 15 | 0 2 1 | 35.46 |
| 2.429 | 5 | 1 0 1 | 36.98 |
| 2.369 | 58 | 1 1 1 | 37.95 |
| 2.307 | 21 | 1 4 0 | 39.00 |
| 2.280 | 2 | 2 0 0 | 39.49 |
| 2.230 | 2 | 2 1 0 | 40.42 |
| 2.212 | 8 | 1 2 1 | 40.76 |
| 2.008 | 6 | 1 3 1 | 45.12 |
| 1.957 | 3 | 0 4 1 | 46.36 |
| 1.937 | 5 | 1 5 0 | 46.86 |
| 1.921 | 1 | 2 3 0 | 47.28 |
| 1.798 | 4 | 1 4 1 | 50.73 |
| 1.783 | 2 | 0 6 0 | 51.18 |
| 1.761 | 13 | 2 1 1 | 51.88 |
| 1.735 | 9 | 2 4 0 | 52.71 |
| 1.693 | 38 | 2 2 1 | 54.11 |
| 1.606 | 26 | 1 5 1 | 57.33 |
| 1.596 | 9 | 2 3 1 | 57.70 |
| 1.560 | 5 | 2 5 0 | 59.16 |
| 1.515 | 13 | 0 6 1 | 61.13 |
| 1.485 | 2 | 2 4 1 | 62.50 |
| 1.462 | 6 | 3 2 0 | 63.58 |
| 1.449 | 7 | 1 7 0 | 64.21 |
| 1.435 | 9 | 0 0 2 | 64.93 |
| 1.405 | 2 | 2 6 0 | 66.51 |
| 1.398 | 4 | 3 3 0 | 66.85 |
| 1.358 | 6 | 1 1 2 | 69.13 |
| 1.343 | 4 | 3 0 1 | 69.98 |
| 1.333 | 2 | 3 1 1 | 70.61 |
| 1.326 | 1 | 1 2 2 | 71.02 |
| 1.303 | 1 | 3 2 1 | 72.49 |
| 1.278 | 6 | 1 3 2 | 74.13 |
| 1.265 | 5 | 0 4 2 | 75.05 |
| 1.262 | 2 | 2 6 1 | 75.25 |
| 1.257 | 3 | 3 3 1 | 75.58 |
| 1.219 | 3 | 1 4 2 | 78.41 |
| 1.214 | 1 | 2 0 2 | 78.73 |
| 1.212 | 3 | 0 8 1 | 78.90 |
| 1.200 | 5 | 3 4 1 | 79.84 |
| 1.161 | 1 | 2 7 1 | 83.12 |
| 1.157 | 2 | 3 6 0 | 83.50 |
| 1.154 | 3 | 2 8 0 | 83.78 |
| 1.153 | 1 | 1 5 2 | 83.83 |
| 1.138 | 1 | 3 5 1 | 85.23 |
| 1.134 | 4 | 4 1 0 | 85.61 |

Manganese oxide hydroxide, groutite, alpha MnOOH – continued

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|--------|--|
| 1.118 | 1 | 0 6 2 | 87.10 |
| 1.106 | 3 | 2 4 2 | 88.30 |
| 1.086 | 1 | 4 3 0 | 90.37 |
| 1.078 | 1 | 3 7 0 | 91.23 |
| 1.073 | 2 | 3 6 1 | 91.77 |
| 1.070 | 1 | 2 8 1 | 92.05 |
| 1.070 | 1 | 0 10 0 | 92.09 |
| 1.068 | 5 | 1 9 1 | 92.33 |
| 1.056 | 2 | 2 5 2 | 93.65 |
| 1.054 | 2 | 2 9 0 | 93.89 |
| 1.024 | 3 | 3 2 2 | 97.55 |
| 1.020 | 4 | 1 7 2 | 98.12 |
| 1.016 | 2 | 4 3 1 | 98.65 |
| 1.006 | 2 | 4 5 0 | 99.92 |
| 1.004 | 1 | 2 6 2 | 100.23 |
| 1.003 | 2 | 0 10 1 | 100.40 |
| 1.001 | 3 | 3 3 2 | 100.55 |
| .979 | 1 | 1 10 1 | 103.75 |
| .969 | 1 | 2 10 0 | 105.35 |
| .951 | 2 | 1 11 0 | 108.13 |
| .948 | 1 | 3 8 1 | 108.73 |
| .942 | 1 | 0 2 3 | 109.76 |
| .933 | 3 | 1 1 3 | 111.35 |
| .901 | 2 | 3 6 2 | 117.58 |
| .899 | 4 | 2 8 2 | 117.90 |
| .899 | 2 | 5 2 0 | 117.92 |
| .890 | 2 | 3 9 1 | 119.82 |
| .890 | 5 | 4 1 2 | 119.98 |
| .879 | 1 | 2 1 3 | 122.36 |
| .871 | 7 | 4 7 1 | 124.40 |
| .870 | 5 | 2 2 3 | 124.49 |
| .869 | 2 | 5 0 1 | 124.80 |
| .866 | 2 | 4 3 2 | 125.64 |
| .862 | 2 | 3 7 2 | 126.71 |
| .858 | 1 | 0 10 2 | 127.79 |
| .858 | 5 | 1 5 3 | 127.79 |
| .856 | 2 | 2 3 3 | 128.18 |
| .854 | 1 | 2 11 1 | 128.79 |
| .852 | 2 | 0 12 1 | 129.54 |
| .850 | 3 | 2 9 2 | 130.10 |
| .843 | 3 | 0 6 3 | 132.05 |
| .837 | 2 | 3 10 1 | 133.96 |
| .827 | 5 | 5 4 1 | 137.44 |
| .824 | 4 | 4 5 2 | 138.46 |
| .823 | 1 | 4 9 0 | 138.82 |
| .823 | 2 | 3 8 2 | 138.87 |

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (alpha HMX) $C_4H_8N_8O_8$

Structure

Orthorhombic, Fdd2 (43), $Z=8$. The structure was determined by Cady et al. [1963].

Lattice parameters

$a=15.14$, $b=23.89$, $c=5.913\text{ \AA}$ [ibid.]

Density (calculated) 1.839 g/cm^3

Thermal parameters

Isotropic: carbon(1) $B=2.731$, carbon(2) $B=2.641$, nitrogen(1) $B=2.093$, nitrogen(2) $B=2.374$, nitrogen(3) $B=2.992$, nitrogen(4) $B=2.900$, oxygen(1) $B=3.587$, oxygen(2) $B=4.234$, oxygen(3) $B=3.003$, oxygen(4) $B=3.658$, hydrogen(3) = 3.60, hydrogens (1), (2), and (4) $B=0.0$

Atomic positions

Erratum: in Cady et al. [op. cit.], $y_{N(1)}$ should be -0.0599 in order to derive the structure factors they give.

Polymorphism

There are 4 known polymorphic forms. The alpha modification described here is stable in the range 103 to 162 °C. [Cady, et al., 1963]

Scattering factors

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

Scale factor

(integrated intensities) 26.64×10^4

Reference

Cady, H.H., Larson, A.C., and Cromer, D.T. (1963).
Acta Cryst. 16, 617.
International Tables for X-ray Crystallography III
(1962). 202.

| $d (\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | $2\theta (\text{ }^\circ)$ $\lambda = 1.54056 \text{ \AA}$ |
|------------------|-----|-----------------------------------|-----|-----|---|
| | | h | k | l | |
| 6.39 | 1 | 2 | 2 | 0 | 13.84 |
| 5.97 | 31 | 0 | 4 | 0 | 14.82 |
| 5.37 | 100 | 1 | 1 | 1 | 16.50 |
| 4.53 | 34 | 1 | 3 | 1 | 19.58 |
| 3.79 | 12 | 4 | 0 | 0 + | 23.48 |
| 3.61 | 45 | 1 | 5 | 1 + | 24.64 |
| 3.52 | 50 | 2 | 6 | 0 | 25.26 |
| 3.46 | 17 | 3 | 3 | 1 | 25.74 |
| 2.986 | 17 | 0 | 8 | 0 + | 29.90 |
| 2.901 | 7 | 1 | 7 | 1 | 30.80 |
| 2.870 | 11 | 0 | 2 | 2 | 31.14 |
| 2.754 | 34 | 2 | 0 | 2 | 32.48 |
| 2.746 | 23 | 4 | 6 | 0 | 32.58 |
| 2.677 | 5 | 5 | 1 | 1 | 33.44 |
| 2.550 | 4 | 3 | 7 | 1 + | 35.16 |
| 2.501 | 1 | 2 | 4 | 2 | 35.88 |
| 2.469 | 6 | 6 | 2 | 0 | 36.36 |
| 2.391 | 2 | 1 | 9 | 1 | 37.58 |
| 2.373 | 8 | 0 | 6 | 2 | 37.88 |
| 2.325 | 3 | 0 | 4 | 0 + | 38.70 |
| 2.287 | 13 | 4 | 2 | 2 | 39.36 |
| 2.281 | 8 | 2 | 10 | 0 | 39.48 |
| 2.265 | 3 | 2 | 6 | 2 | 39.76 |
| 2.183 | 4 | 3 | 9 | 1 | 41.32 |
| 2.170 | 3 | 4 | 4 | 2 | 41.58 |
| 2.115 | 1 | 5 | 7 | 1 | 42.72 |
| 2.024 | 1 | 7 | 1 | 1 | 44.74 |
| 2.021 | 2 | 1 | 11 | 1 | 44.82 |
| 1.991 | 1 | 0 | 12 | 0 | 45.52 |
| 1.968 | 1 | 7 | 3 | 1 | 46.08 |
| 1.948 | 3 | 1 | 1 | 3 | 46.58 |
| 1.926 | 2 | 2 | 12 | 0 | 47.16 |
| 1.898 | 2 | 1 | 3 | 3 | 47.88 |
| 1.892 | 2 | 5 | 9 | 1 | 48.06 |
| 1.809 | 1 | 1 | 5 | 3 | 50.40 |
| 1.804 | 1 | 8 | 4 | 0 | 50.54 |
| 1.743 | 1 | 1 | 13 | 1 | 52.44 |
| 1.714 | 1 | 3 | 5 | 3 | 53.42 |
| 1.691 | 1 | 5 | 11 | 1 | 54.18 |
| 1.658 | 1 | 3 | 13 | 1 | 55.38 |
| 1.614 | 3 | 2 | 12 | 2 + | 57.02 |
| 1.580 | 1 | 8 | 2 | 2 | 58.36 |
| 1.540 | 2 | 8 | 4 | 2 | 60.02 |
| 1.484 | 1 | 7 | 11 | 1 | 62.56 |

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (alpha HMX) $C_4H_8N_8O_8$ – continued

| Calculated Pattern (Integrated) | | | |
|---------------------------------|-----|--------|--|
| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
| 6.39 | 1 | 2 2 0 | 13.84 |
| 5.97 | 30 | 0 4 0 | 14.82 |
| 5.37 | 100 | 1 1 1 | 16.50 |
| 4.53 | 35 | 1 3 1 | 19.58 |
| 3.79 | 4 | 3 1 1 | 23.45 |
| 3.78 | 10 | 4 0 0 | 23.48 |
| 3.61 | 48 | 1 5 1 | 24.65 |
| 3.61 | 3 | 4 2 0 | 24.65 |
| 3.52 | 56 | 2 6 0 | 25.25 |
| 3.46 | 18 | 3 3 1 | 25.74 |
| 2.993 | 4 | 3 5 1 | 29.83 |
| 2.986 | 18 | 0 8 0 | 29.90 |
| 2.901 | 8 | 1 7 1 | 30.80 |
| 2.870 | 13 | 0 2 2 | 31.14 |
| 2.754 | 40 | 2 0 2 | 32.48 |
| 2.743 | 8 | 4 6 0 | 32.61 |
| 2.684 | 1 | 2 2 2 | 33.36 |
| 2.678 | 5 | 5 1 1 | 33.43 |
| 2.553 | 1 | 5 3 1 | 35.12 |
| 2.551 | 4 | 3 7 1 | 35.16 |
| 2.501 | 1 | 2 4 2 | 35.88 |
| 2.469 | 7 | 0 2 0 | 36.36 |
| 2.391 | 3 | 1 9 1 | 37.58 |
| 2.374 | 10 | 0 0 2 | 37.87 |
| 2.347 | 4 | 5 5 1 | 38.31 |
| 2.344 | 1 | 4 8 0 | 38.36 |
| 2.324 | 4 | 0 4 0 | 38.71 |
| 2.287 | 17 | 4 2 2 | 39.37 |
| 2.278 | 3 | 2 10 0 | 39.52 |
| 2.265 | 3 | 2 6 2 | 39.76 |
| 2.183 | 5 | 3 9 1 | 41.32 |
| 2.171 | 4 | 4 4 2 | 41.57 |
| 2.115 | 1 | 5 7 1 | 42.71 |
| 2.024 | 1 | 7 1 1 | 44.74 |
| 2.020 | 1 | 1 11 1 | 44.82 |
| 1.991 | 2 | 0 12 0 | 45.53 |
| 1.968 | 1 | 7 3 1 | 46.08 |
| 1.948 | 4 | 1 1 3 | 46.58 |
| 1.925 | 2 | 2 12 0 | 47.17 |
| 1.898 | 2 | 1 3 3 | 47.88 |
| 1.891 | 2 | 5 9 1 | 48.07 |
| 1.809 | 1 | 1 5 3 | 50.40 |
| 1.804 | 1 | 8 4 0 | 50.55 |
| 1.762 | 1 | 4 12 0 | 51.85 |
| 1.743 | 1 | 1 13 1 | 52.45 |
| 1.714 | 2 | 3 5 3 | 53.42 |
| 1.691 | 1 | 5 11 1 | 54.19 |
| 1.658 | 1 | 3 13 1 | 55.38 |
| 1.648 | 1 | 5 1 3 | 55.73 |
| 1.615 | 2 | 0 8 2 | 56.99 |

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|--------|--|
| 1.614 | 1 | 9 1 1 | 57.00 |
| 1.613 | 2 | 2 12 2 | 57.03 |
| 1.586 | 1 | 9 3 1 | 58.13 |
| 1.580 | 1 | 8 2 2 | 58.36 |
| 1.540 | 3 | 8 4 2 | 60.02 |
| 1.518 | 1 | 5 13 1 | 60.97 |
| 1.484 | 1 | 7 11 1 | 62.56 |
| 1.440 | 1 | 2 2 4 | 64.66 |
| 1.377 | 1 | 4 0 4 | 68.03 |
| 1.320 | 1 | 5 17 1 | 71.42 |

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (beta HMX) $C_4H_8N_8O_8$

Structure

Monoclinic, $P2_1/n$ (14), $Z=2$. The structure was determined first by Eiland and Pepinsky [1955]. Cady, Larson, and Cromer [1963] used Eiland's and Pepinsky's data and did a least squares refinement with anisotropic temperature factors, but did not determine the hydrogen positions. Choi and Boutin [1970] collected new 3-dimensional data from neutron diffraction analysis and refined parameters for all atoms including hydrogen.

Lattice parameters

$a=6.54$, $b=11.05$, $c=7.37\text{\AA}$, $\beta=102.8^\circ$ [Eiland and Pepinsky, 1955]

Density
(calculated) 1.89 g/cm^3

Thermal parameters

Isotropic:hydrogen(1):B=2.892;hydrogen(2):B=2.726
hydrogen(3):B=2.790;hydrogen(4):B=3.686 [Choi and Boutin, 1970]. Nitrogen(1):B=1.616; nitrogen(2):B=1.468;nitrogen(3):B=1.361;nitrogen(4):B=1.676
oxygen(1):B=2.282; oxygen(2):B=2.769; oxygen(3):B=3.063; oxygen(4):B=2.523; carbon(1):B=1.294; carbon(2):B=1.600.

Atomic positions

Choi and Boutin [1970]

Polymorphism

There are 4 known polymorphic forms. The beta modification described here is the stable form at room temperature [Cady et al., 1963].

Scattering factors

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

Scale factor

(Integrated intensities) 1.303×10^4

Additional patterns

1. PDF card 3-0225 [Soldate and Noyes, 1947]

Reference

Cady, H.H., Larson, A.C., and Cromer, D.T. (1963).

Acta Cryst. **16**, 617.

Choi, C.S. and Boutin, H.P. (1970). Acta Cryst. **B26**, 1235.

Eiland, P.F. and Pepinsky, R. (1955). Z. Krist. **106**, 18.

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

Soldate, A.M. and Noyes, R.M. (1947). Anal. Chem. **19**, 442.

| $d (\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | | $2\theta (\text{ }^\circ)$ $\lambda = 1.54056 \text{\AA}$ |
|------------------|-----|-----------------------------------|-----|-----|-------|--|
| | | h | k | l | \pm | |
| 6.02 | 39 | 0 | 1 | 1 | | 14.70 |
| 5.52 | 40 | 1 | 1 | 0 | + | 16.04 |
| 5.40 | 2 | -1 | 0 | 1 | | 16.40 |
| 4.85 | 11 | -1 | 1 | 1 | | 18.26 |
| 4.32 | 100 | 1 | 0 | 1 | | 20.56 |
| 4.02 | 8 | 1 | 1 | 1 | | 22.08 |
| 3.86 | 53 | -1 | 2 | 1 | | 23.00 |
| 3.59 | 1 | 0 | 0 | 2 | | 24.76 |
| 3.42 | 7 | 0 | 1 | 2 | | 26.06 |
| 3.40 | 23 | 1 | 2 | 1 | | 26.18 |
| 3.32 | 9 | -1 | 1 | 2 | | 26.84 |
| 3.28 | 28 | 0 | 3 | 1 | | 27.18 |
| 3.19 | 12 | 1 | 3 | 0 | + | 27.96 |
| 3.06 | 13 | -2 | 1 | 1 | + | 29.12 |
| 3.04 | 6 | -1 | 3 | 1 | | 29.32 |
| 3.01 | 33 | 0 | 2 | 2 | | 29.64 |
| 2.94 | 4 | -1 | 2 | 2 | | 30.34 |
| 2.80 | 77 | 1 | 3 | 1 | | 31.92 |
| 2.76 | 7 | 0 | 4 | 0 | + | 32.38 |
| 2.70 | 3 | -2 | 0 | 2 | | 33.14 |
| 2.62 | 1 | 2 | 1 | 1 | | 34.16 |
| 2.57 | 1 | 0 | 3 | 2 | | 34.86 |
| 2.53 | 4 | 1 | 4 | 0 | | 35.38 |
| 2.46 | 2 | -1 | 4 | 1 | | 36.50 |
| 2.43 | 7 | -2 | 2 | 2 | + | 37.02 |
| 2.41 | 8 | 2 | 3 | 0 | + | 37.26 |
| 2.26 | 3 | 1 | 3 | 2 | | 39.78 |
| 2.22 | 1 | -1 | 2 | 3 | | 40.56 |
| 2.197 | 2 | 0 | 2 | 3 | | 41.04 |
| 2.190 | 8 | 0 | 4 | 2 | | 41.18 |
| 2.178 | 4 | -2 | 3 | 2 | + | 41.42 |
| 2.158 | 2 | 2 | 0 | 2 | | 41.82 |
| 2.133 | 4 | -3 | 1 | 1 | | 42.34 |
| 2.119 | 2 | -2 | 1 | 3 | + | 42.64 |
| 2.113 | 2 | 0 | 5 | 1 | | 42.76 |
| 2.088 | 5 | 2 | 4 | 0 | + | 43.30 |
| 2.027 | 1 | -1 | 3 | 3 | | 44.68 |
| 2.010 | 3 | 2 | 2 | 2 | + | 45.06 |
| 1.984 | 2 | 3 | 2 | 0 | | 45.70 |
| 1.958 | 2 | 1 | 2 | 3 | | 46.32 |
| 1.926 | 2 | 3 | 0 | 1 | | 47.16 |
| 1.913 | 1 | -3 | 2 | 2 | | 47.50 |
| 1.897 | 2 | 3 | 1 | 1 | | 47.92 |
| 1.883 | 1 | 0 | 5 | 2 | | 48.30 |
| 1.872 | 2 | -3 | 3 | 1 | | 48.60 |
| 1.862 | 3 | 2 | 3 | 2 | + | 48.86 |
| 1.842 | 1 | 0 | 6 | 0 | | 49.44 |
| 1.817 | 2 | -2 | 5 | 1 | | 50.18 |
| 1.810 | 1 | 0 | 4 | 3 | | 50.38 |
| 1.801 | 4 | -3 | 0 | 3 | | 50.64 |

Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (beta HMX) $C_4H_8N_8O_8$ – continued

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|---------|--|
| 1.796 | 4 | 0 0 4 | 50.78 |
| 1.769 | 1 | 1 6 0 | 51.62 |
| 1.739 | 1 | -2 0 4 | 52.58 |
| 1.710 | 1 | 2 5 1 | 53.54 |
| 1.685 | 1 | 3 4 0 | 54.42 |
| 1.669 | 2 | 1 4 3 | 54.96 |
| 1.659 | 1 | -2 2 4 | 55.34 |
| 1.627 | 1 | -1 6 2 | 56.50 |
| 1.615 | 1 | 0 3 4 | 56.98 |
| 1.594 | 1 | -4 0 2 | 57.78 |
| 1.578 | 1 | -4 1 2 | 58.44 |
| 1.573 | 1 | -2 3 4 | 58.64 |
| 1.550 | 3 | 1 6 2 + | 59.60 |
| 1.521 | 1 | 2 6 1 | 60.84 |
| 1.467 | 1 | -1 6 3 | 63.34 |

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|--------|--|
| 2.26 | 4 | 1 3 2 | 39.79 |
| 2.22 | 1 | -1 2 3 | 40.56 |
| 2.198 | 2 | 0 2 3 | 41.03 |
| 2.190 | 9 | 0 4 2 | 41.18 |
| 2.178 | 4 | -2 3 2 | 41.42 |
| 2.178 | 1 | 2 3 1 | 41.43 |
| 2.159 | 2 | 2 0 2 | 41.81 |
| 2.133 | 5 | -3 1 1 | 42.34 |
| 2.119 | 1 | -2 1 3 | 42.62 |
| 2.119 | 1 | 2 1 2 | 42.64 |
| 2.112 | 1 | 0 5 1 | 42.77 |
| 2.088 | 1 | -2 4 1 | 43.30 |
| 2.088 | 4 | 2 4 0 | 43.30 |
| 2.027 | 1 | -1 3 3 | 44.68 |
| 2.011 | 4 | 2 2 2 | 45.05 |
| 2.008 | 2 | 0 3 3 | 45.11 |
| 1.984 | 2 | 3 2 0 | 45.70 |
| 1.959 | 2 | 1 2 3 | 46.32 |
| 1.925 | 2 | 3 0 1 | 47.17 |
| 1.913 | 1 | -3 2 2 | 47.50 |
| 1.897 | 3 | 3 1 1 | 47.92 |
| 1.882 | 1 | 0 5 2 | 48.31 |
| 1.872 | 3 | -3 3 1 | 48.59 |
| 1.863 | 1 | -2 3 3 | 48.85 |
| 1.862 | 3 | 2 3 2 | 48.86 |
| 1.842 | 2 | 0 6 0 | 49.45 |
| 1.816 | 1 | -2 5 1 | 50.18 |
| 1.810 | 1 | 0 4 3 | 50.38 |
| 1.801 | 5 | -3 0 3 | 50.65 |
| 1.797 | 2 | 0 0 4 | 50.77 |
| 1.769 | 2 | 1 6 0 | 51.61 |
| 1.743 | 1 | -1 6 1 | 52.45 |
| 1.739 | 1 | -2 0 4 | 52.58 |
| 1.710 | 1 | 2 5 1 | 53.54 |
| 1.685 | 1 | 3 4 0 | 54.42 |
| 1.669 | 3 | 1 4 3 | 54.97 |
| 1.659 | 1 | -2 2 4 | 55.33 |
| 1.628 | 2 | -1 6 2 | 56.49 |
| 1.615 | 1 | 0 3 4 | 56.98 |
| 1.594 | 1 | -4 0 2 | 57.78 |
| 1.578 | 1 | -4 1 2 | 58.43 |
| 1.573 | 1 | -2 3 4 | 58.65 |
| 1.550 | 3 | 1 6 2 | 59.60 |
| 1.550 | 2 | -3 5 1 | 59.61 |
| 1.522 | 1 | 2 6 1 | 60.83 |
| 1.467 | 2 | -1 6 3 | 63.34 |
| 1.463 | 1 | -4 3 2 | 63.53 |
| 1.452 | 1 | 3 5 1 | 64.09 |
| 1.401 | 2 | 2 6 2 | 66.70 |
| 1.354 | 1 | -3 4 4 | 69.37 |

Calculated Pattern (Integrated)

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|--------|--|
| 6.02 | 36 | 0 1 1 | 14.69 |
| 5.52 | 14 | 0 2 0 | 16.03 |
| 5.52 | 24 | 1 1 0 | 16.03 |
| 5.40 | 1 | -1 0 1 | 16.39 |
| 4.85 | 11 | -1 1 1 | 18.26 |
| 4.32 | 100 | 1 0 1 | 20.55 |
| 4.02 | 9 | 1 1 1 | 22.09 |
| 3.86 | 57 | -1 2 1 | 23.00 |
| 3.59 | 1 | 0 0 2 | 24.76 |
| 3.42 | 6 | 0 1 2 | 26.05 |
| 3.40 | 24 | 1 2 1 | 26.17 |
| 3.32 | 10 | -1 1 2 | 26.85 |
| 3.28 | 30 | 0 3 1 | 27.18 |
| 3.19 | 8 | 1 3 0 | 27.95 |
| 3.19 | 5 | 2 0 0 | 27.96 |
| 3.06 | 10 | -2 1 1 | 29.12 |
| 3.06 | 4 | 2 1 0 | 29.13 |
| 3.04 | 5 | -1 3 1 | 29.32 |
| 3.01 | 38 | 0 2 2 | 29.63 |
| 2.94 | 5 | -1 2 2 | 30.34 |
| 2.80 | 92 | 1 3 1 | 31.91 |
| 2.76 | 5 | 0 4 0 | 32.38 |
| 2.76 | 2 | 2 2 0 | 32.39 |
| 2.70 | 4 | -2 0 2 | 33.14 |
| 2.62 | 1 | 2 1 1 | 34.15 |
| 2.57 | 1 | 0 3 2 | 34.85 |
| 2.53 | 4 | 1 4 0 | 35.38 |
| 2.46 | 2 | -1 4 1 | 36.50 |
| 2.43 | 2 | -1 0 3 | 37.01 |
| 2.43 | 7 | -2 2 2 | 37.01 |
| 2.41 | 1 | -2 3 1 | 37.27 |
| 2.41 | 9 | 2 3 0 | 37.27 |

Potassium zinc bromide hydrate, $\text{KZnBr}_3 \cdot 2\text{H}_2\text{O}$

Structure

Orthorhombic, $P2_12_12_1$ (19), $Z=4$. The structure was determined by Holinski [1967].

Lattice parameters

$a=9.327(2)$, $b=13.067(4)$, $c=6.786(2)\text{\AA}$ [ibid]

Density

(calculated) 3.053 g/cm^3

Thermal parameters

Isotropic: bromine(1): $B=2.86$; bromine(2): $B=2.97$
bromine(3): $B=2.86$; zinc: $B=2.28$; potassium: $B=3.51$
water(1): $B=2.58$; water(2): $B=3.31$.

Atomic positions

To conform to the symmetry arrangements used in the International Tables I [1952], the values for the x parameters were replaced by $-x$. The value for $x_{\text{Br}(1)}$ should be -0.0129 in order to derive structure factors given by Holinski [op. cit.].

Scattering factors

O^0 , K^+ , Zn^{2+} [International Tables, 1962]
 Br^- [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 12.89×10^4

Reference

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
Holinski, R. (1967). Dissertation, Technischen Hochschule, 3392 Clausthal-Zellerfeld, W. Germany.

| $d (\text{\AA})$ | I | Calculated Pattern (Peak heights) | | | $2\theta (^{\circ})$ $\lambda = 1.54056 \text{\AA}$ |
|------------------|-----|-----------------------------------|-----|-----|--|
| | | h | k | l | |
| 7.58 | 6 | 1 | 1 | 0 | 11.66 |
| 6.53 | 18 | 0 | 2 | 0 | 13.54 |
| 6.02 | 14 | 0 | 1 | 1 | 14.70 |
| 5.49 | 47 | 1 | 0 | 1 | 16.14 |
| 5.35 | 11 | 1 | 2 | 0 | 16.56 |
| 5.06 | 13 | 1 | 1 | 1 | 17.52 |
| 4.706 | 21 | 0 | 2 | 1 | 18.84 |
| 4.392 | 1 | 2 | 1 | 0 | 20.20 |
| 4.203 | 4 | 1 | 2 | 1 | 21.12 |
| 3.844 | 32 | 2 | 0 | 1 | 23.12 |
| 3.795 | 2 | 2 | 2 | 0 | 23.42 |
| 3.687 | 5 | 2 | 1 | 1 | 24.12 |
| 3.666 | 4 | 0 | 3 | 1 | 24.26 |
| 3.411 | 63 | 1 | 3 | 1 | 26.10 |
| 3.312 | 5 | 2 | 2 | 1 | 26.90 |
| 3.283 | 13 | 0 | 1 | 2 | 27.14 |
| 3.184 | 100 | 1 | 0 | 2 | 28.00 |
| 3.097 | 5 | 1 | 1 | 2 | 28.80 |
| 3.089 | 3 | 1 | 4 | 0 | 28.88 |
| 3.023 | 2 | 3 | 1 | 0 | 29.52 |
| 2.944 | 1 | 0 | 4 | 1 | 30.34 |
| 2.882 | 48 | 2 | 3 | 1 | 31.00 |
| 2.826 | 28 | 3 | 0 | 1 | 31.64 |
| 2.763 | 2 | 3 | 1 | 1 | 32.38 |
| 2.743 | 1 | 2 | 0 | 2 | 32.62 |
| 2.685 | 7 | 2 | 1 | 2 | 33.34 |
| 2.676 | 5 | 2 | 4 | 0 | 33.46 |
| 2.595 | 2 | 3 | 2 | 1 | 34.54 |
| 2.573 | 14 | 1 | 3 | 2 | 34.84 |
| 2.489 | 3 | 2 | 4 | 1 | 36.06 |
| 2.371 | 4 | 3 | 3 | 1 | 37.92 |
| 2.360 | 1 | 1 | 5 | 1 | 38.10 |
| 2.321 | 3 | 2 | 3 | 2 | 38.76 |
| 2.292 | 3 | 3 | 0 | 2 | 39.28 |
| 2.285 | 2 | 1 | 4 | 2 | 39.40 |
| 2.252 | 2 | 3 | 4 | 0 | 40.00 |
| 2.205 | 6 | 4 | 0 | 1 | 40.90 |
| 2.198 | 5 | 1 | 0 | 3 | 41.02 |
| 2.178 | 20 | 0 | 6 | 0 | 41.42 |
| 2.171 | 12 | 1 | 1 | 3 | 41.56 |
| 2.161 | 3 | 2 | 5 | 1 | 41.76 |
| 2.138 | 2 | 3 | 4 | 1 | 42.24 |
| 2.083 | 1 | 1 | 2 | 3 | 43.40 |
| 2.071 | 1 | 0 | 5 | 2 | 43.68 |
| 2.055 | 10 | 4 | 3 | 0 | 44.02 |
| 2.035 | 10 | 2 | 0 | 3 | 44.48 |
| 2.028 | 30 | 3 | 3 | 2 | 44.64 |
| 2.024 | 20 | 1 | 6 | 1 | 44.74 |
| 2.008 | 4 | 0 | 3 | 3 | 45.12 |
| 2.002 | 3 | 3 | 5 | 0 | 45.26 |

Potassium zinc bromide hydrate, $KZnBr_3 \cdot 2H_2O$ – continued

| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|---------|--|
| 1.967 | 8 | 4 3 1 | 46.10 |
| 1.963 | 5 | 1 3 3 | 46.22 |
| 1.943 | 3 | 2 2 3 | 46.70 |
| 1.919 | 1 | 3 5 1 | 47.34 |
| 1.901 | 1 | 4 1 2 | 47.80 |
| 1.895 | 6 | 2 6 1 + | 47.98 |
| 1.844 | 11 | 2 3 3 + | 49.38 |
| 1.833 | 1 | 0 6 2 | 49.70 |
| 1.828 | 2 | 4 4 1 + | 49.84 |
| 1.811 | 1 | 3 1 3 | 50.34 |
| 1.798 | 14 | 1 6 2 + | 50.72 |
| 1.767 | 2 | 1 7 1 | 51.68 |
| 1.758 | 1 | 4 3 2 | 51.96 |
| 1.740 | 1 | 4 5 0 | 52.56 |
| 1.734 | 2 | 5 2 1 | 52.74 |
| 1.725 | 7 | 3 6 1 + | 53.04 |
| 1.697 | 5 | 0 4 | 54.00 |
| 1.686 | 2 | 4 5 1 + | 54.38 |
| 1.682 | 2 | 0 1 4 | 54.50 |
| 1.669 | 1 | 1 0 4 | 54.98 |
| 1.663 | 11 | 5 3 1 | 55.20 |
| 1.658 | 6 | 4 4 2 + | 55.38 |
| 1.635 | 2 | 0 7 2 + | 56.20 |
| 1.624 | 3 | 4 0 3 | 56.64 |
| 1.611 | 1 | 1 7 2 | 57.14 |
| 1.609 | 1 | 1 8 0 | 57.20 |
| 1.606 | 1 | 2 5 3 | 57.32 |
| 1.588 | 1 | 0 8 1 | 58.04 |
| 1.579 | 1 | 3 6 2 | 58.40 |
| 1.575 | 2 | 5 4 1 + | 58.54 |
| 1.566 | 1 | 1 8 1 | 58.94 |
| 1.559 | 1 | 1 3 4 | 59.24 |
| 1.555 | 3 | 6 0 0 | 59.40 |
| 1.549 | 3 | 4 6 1 + | 59.62 |
| 1.530 | 1 | 5 3 2 | 60.44 |
| 1.521 | 3 | 4 3 3 | 60.84 |
| 1.518 | 2 | 5 5 0 | 61.00 |
| 1.497 | 3 | 2 3 4 + | 61.92 |
| 1.487 | 3 | 2 6 3 | 62.40 |
| 1.462 | 1 | 5 4 2 | 63.60 |
| 1.454 | 1 | 4 4 3 + | 63.98 |
| 1.431 | 1 | 6 3 1 + | 65.12 |
| 1.423 | 1 | 0 5 4 | 65.54 |
| 1.409 | 1 | 3 3 4 | 66.28 |
| 1.404 | 2 | 1 9 1 + | 66.56 |
| 1.386 | 2 | 2 9 0 + | 67.50 |
| 1.367 | 2 | 5 3 3 | 68.62 |
| 1.358 | 1 | 2 9 1 | 69.10 |
| 1.355 | 1 | 3 4 4 | 69.30 |
| 1.338 | 3 | 0 6 4 | 70.28 |

| Calculated Pattern (Integrated) | | | |
|---------------------------------|-----|-------|--|
| d (Å) | I | hkl | 2θ (°) $\lambda = 1.54056 \text{ Å}$ |
| 7.59 | 7 | 1 1 0 | 11.65 |
| 6.53 | 22 | 0 2 0 | 13.54 |
| 6.02 | 17 | 0 1 1 | 14.70 |
| 5.49 | 59 | 1 0 1 | 16.14 |
| 5.35 | 14 | 1 2 0 | 16.55 |
| 5.06 | 16 | 1 1 1 | 17.51 |
| 4.707 | 27 | 0 2 1 | 18.84 |
| 4.392 | 1 | 2 1 0 | 20.20 |
| 4.202 | 5 | 1 2 1 | 21.13 |
| 3.843 | 45 | 2 0 1 | 23.12 |
| 3.796 | 1 | 2 2 0 | 23.42 |
| 3.687 | 6 | 2 1 1 | 24.12 |
| 3.666 | 5 | 0 3 1 | 24.26 |
| 3.412 | 91 | 1 3 1 | 26.10 |
| 3.393 | 4 | 0 0 2 | 26.24 |
| 3.183 | 87 | 2 3 0 | 28.01 |
| 3.098 | 7 | 1 1 2 | 28.80 |
| 3.313 | 6 | 2 2 1 | 26.89 |
| 3.284 | 19 | 0 1 2 | 27.13 |
| 3.189 | 100 | 1 0 2 | 27.96 |
| 3.083 | 1 | 1 4 0 | 28.94 |
| 3.025 | 3 | 3 1 0 | 29.51 |
| 2.943 | 2 | 0 4 1 | 30.34 |
| 2.882 | 75 | 2 3 1 | 31.01 |
| 2.866 | 3 | 1 2 2 | 31.19 |
| 2.826 | 46 | 3 0 1 | 31.63 |
| 2.763 | 2 | 3 1 1 | 32.38 |
| 2.744 | 2 | 2 0 2 | 32.61 |
| 2.685 | 10 | 2 1 2 | 33.34 |
| 2.676 | 4 | 2 4 0 | 33.46 |
| 2.594 | 3 | 3 2 1 | 34.55 |
| 2.573 | 22 | 1 3 2 | 34.84 |
| 2.530 | 1 | 2 2 2 | 35.46 |
| 2.489 | 5 | 2 4 1 | 36.05 |
| 2.371 | 6 | 3 3 1 | 37.92 |
| 2.359 | 2 | 1 5 1 | 38.11 |
| 2.321 | 4 | 2 3 2 | 38.76 |
| 2.292 | 4 | 3 0 2 | 39.27 |
| 2.282 | 1 | 1 4 2 | 39.46 |
| 2.252 | 3 | 3 4 0 | 40.00 |
| 2.229 | 1 | 0 1 3 | 40.44 |
| 2.205 | 10 | 4 0 1 | 40.89 |
| 2.198 | 2 | 1 0 3 | 41.02 |
| 2.178 | 34 | 0 6 0 | 41.43 |
| 2.174 | 1 | 4 1 1 | 41.49 |
| 2.168 | 1 | 1 1 3 | 41.63 |
| 2.163 | 1 | 3 2 2 | 41.72 |
| 2.161 | 3 | 2 5 1 | 41.76 |
| 2.138 | 1 | 0 2 3 | 42.24 |
| 2.137 | 3 | 3 4 1 | 42.25 |

Potassium zinc bromide hydrate, $\text{KZnBr}_3 \cdot 2\text{H}_2\text{O}$ – continued

| d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ | d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ |
|----------------------|-----|-------|--|----------------------|-----|-------|--|
| 2.089 | 1 | 4 2 1 | 43.27 | 1.611 | 1 | 1 7 2 | 57.13 |
| 2.083 | 2 | 1 2 3 | 43.39 | 1.609 | 1 | 1 8 0 | 57.21 |
| 2.070 | 1 | 0 5 2 | 43.68 | 1.606 | 1 | 2 5 3 | 57.33 |
| 2.056 | 17 | 4 3 0 | 44.01 | 1.588 | 2 | 0 8 1 | 58.03 |
| 2.035 | 13 | 2 0 3 | 44.48 | 1.579 | 2 | 3 6 2 | 58.40 |
| 2.028 | 48 | 3 3 2 | 44.63 | 1.576 | 1 | 4 2 3 | 58.53 |
| 2.024 | 6 | 1 6 1 | 44.73 | 1.576 | 2 | 5 4 1 | 58.53 |
| 2.021 | 1 | 1 5 2 | 44.80 | 1.565 | 1 | 1 8 1 | 58.95 |
| 2.011 | 2 | 2 1 3 | 45.04 | 1.559 | 1 | 1 3 4 | 59.24 |
| 2.007 | 6 | 0 3 3 | 45.13 | 1.554 | 5 | 6 0 0 | 59.41 |
| 2.001 | 1 | 3 5 0 | 45.29 | 1.550 | 3 | 4 6 1 | 59.62 |
| 1.967 | 13 | 4 3 1 | 46.10 | 1.549 | 1 | 2 2 4 | 59.65 |
| 1.963 | 2 | 1 3 3 | 46.22 | 1.548 | 2 | 4 5 2 | 59.67 |
| 1.943 | 6 | 2 2 3 | 46.71 | 1.547 | 1 | 1 6 3 | 59.72 |
| 1.919 | 2 | 3 5 1 | 47.33 | 1.530 | 2 | 5 3 2 | 60.44 |
| 1.901 | 2 | 4 1 2 | 47.80 | 1.521 | 6 | 4 3 3 | 60.84 |
| 1.898 | 1 | 4 4 0 | 47.89 | 1.518 | 1 | 5 5 0 | 60.97 |
| 1.895 | 8 | 2 6 1 | 47.97 | 1.499 | 2 | 3 5 3 | 61.86 |
| 1.892 | 6 | 2 5 2 | 48.04 | 1.497 | 6 | 2 3 4 | 61.93 |
| 1.876 | 1 | 3 4 2 | 48.47 | 1.487 | 6 | 2 6 3 | 62.40 |
| 1.847 | 1 | 5 1 0 | 49.31 | 1.462 | 2 | 5 4 2 | 63.60 |
| 1.844 | 19 | 2 3 3 | 49.39 | 1.454 | 1 | 4 4 3 | 63.98 |
| 1.833 | 1 | 0 6 2 | 49.70 | 1.454 | 1 | 1 8 2 | 63.99 |
| 1.830 | 1 | 1 7 0 | 49.77 | 1.433 | 1 | 2 4 4 | 65.04 |
| 1.829 | 1 | 3 0 3 | 49.81 | 1.431 | 2 | 6 3 1 | 65.13 |
| 1.828 | 2 | 4 4 1 | 49.85 | 1.423 | 1 | 0 5 4 | 65.55 |
| 1.811 | 1 | 3 1 3 | 50.33 | 1.409 | 2 | 3 3 4 | 66.27 |
| 1.800 | 2 | 0 7 1 | 50.68 | 1.404 | 2 | 1 9 1 | 66.57 |
| 1.799 | 4 | 5 0 1 | 50.71 | 1.403 | 1 | 2 8 2 | 66.57 |
| 1.798 | 22 | 1 6 2 | 50.72 | 1.387 | 2 | 5 6 1 | 67.48 |
| 1.767 | 3 | 1 7 1 | 51.68 | 1.386 | 2 | 2 9 0 | 67.51 |
| 1.758 | 1 | 4 3 2 | 51.97 | 1.376 | 1 | 2 7 3 | 68.10 |
| 1.740 | 1 | 4 5 0 | 52.56 | 1.367 | 3 | 5 3 3 | 68.62 |
| 1.734 | 2 | 5 2 1 | 52.74 | 1.358 | 3 | 2 9 1 | 69.10 |
| 1.727 | 5 | 2 4 3 | 52.96 | 1.355 | 2 | 3 4 4 | 69.28 |
| 1.725 | 11 | 3 6 1 | 53.04 | 1.343 | 1 | 1 0 5 | 69.99 |
| 1.723 | 3 | 3 5 2 | 53.10 | 1.338 | 6 | 0 6 4 | 70.28 |
| 1.706 | 1 | 2 6 2 | 53.69 | 1.325 | 1 | 1 6 4 | 71.10 |
| 1.697 | 10 | 0 0 4 | 54.01 | 1.311 | 1 | 1 8 3 | 71.96 |
| 1.686 | 1 | 3 3 3 | 54.36 | 1.308 | 3 | 4 3 4 | 72.13 |
| 1.685 | 1 | 4 5 1 | 54.39 | 1.307 | 1 | 7 0 1 | 72.19 |
| 1.682 | 1 | 0 1 4 | 54.50 | 1.302 | 3 | 4 6 3 | 72.56 |
| 1.669 | 2 | 1 0 4 | 54.97 | 1.283 | 3 | 1 3 5 | 73.76 |
| 1.662 | 21 | 5 3 1 | 55.20 | 1.2739 | 1 | 2 8 3 | 74.41 |
| 1.656 | 1 | 4 4 2 | 55.43 | 1.2652 | 3 | 6 6 0 | 75.01 |
| 1.656 | 1 | 1 1 4 | 55.45 | 1.2485 | 1 | 2 3 5 | 76.19 |
| 1.636 | 3 | 0 7 2 | 56.19 | 1.2438 | 2 | 3 0 5 | 76.53 |
| 1.635 | 1 | 5 0 2 | 56.23 | 1.2402 | 5 | 7 0 2 | 76.79 |
| 1.633 | 1 | 0 8 0 | 56.27 | 1.2325 | 1 | 4 9 0 | 77.36 |
| 1.624 | 6 | 4 0 3 | 56.65 | 1.2291 | 3 | 6 3 3 | 77.62 |

Potassium zinc iodide hydrate, $KZnI_3 \cdot 2H_2O$

Structure

Orthorhombic, $P2_12_12_1$ (19), $Z=4$. The structure was determined by Holinski [private comm., 1973].

Lattice parameters

$a=9.950(3)$, $b=13.727(4)$, $c=7.072(2)\text{\AA}$; published value: $b=13.726$ [ibid]

Density
(calculated) 3.584 g/cm^3

Thermal parameters

Isotropic [Holinski, op. cit.]

Scattering factors

O^0 , K^+ , Zn^{2+} [International Tables, 1962]
 I^- [Cromer and Waber, 1965]

Scale factor

(integrated intensities) 36.27×10^4

Reference

Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. 18, 104.
Holinski, R., Dissertation, 1967; Technischen Hochschule, 3392 Clausthal-Zellerfeld, W. Germany.
International Tables for X-ray Crystallography, III 1962, pgs. 202,204.

| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|---------|----------------------|---------------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (^{\circ})$ | $\lambda = 1.54056 \text{ \AA}$ |
| 8.05 | 4 | 1 1 0 | 10.98 | |
| 6.86 | 10 | 0 2 0 | 12.90 | |
| 6.28 | 6 | 0 1 1 | 14.08 | |
| 5.76 | 61 | 1 0 1 | 15.36 | |
| 5.65 | 7 | 1 2 0 | 15.68 | |
| 5.31 | 8 | 1 1 1 | 16.68 | |
| 4.973 | 6 | 2 0 0 | 17.82 | |
| 4.924 | 14 | 0 2 1 | 18.00 | |
| 4.414 | 2 | 1 2 1 | 20.10 | |
| 4.070 | 46 | 2 0 1 | 21.82 | |
| 3.900 | 4 | 2 1 1 | 22.78 | |
| 3.841 | 18 | 0 3 1 | 23.14 | |
| 3.584 | 100 | 1 3 1 | 24.82 | |
| 3.537 | 7 | 0 0 2 | 25.16 | |
| 3.501 | 3 | 2 2 1 | 25.42 | |
| 3.424 | 9 | 0 1 2 | 26.00 | |
| 3.368 | 79 | 2 3 0 | 26.44 | |
| 3.331 | 88 | 1 0 2 | 26.74 | |
| 3.238 | 2 | 1 1 2 | 27.52 | |
| 3.225 | 3 | 3 1 0 | 27.64 | |
| 3.087 | 2 | 0 4 1 | 28.90 | |
| 3.040 | 45 | 2 3 1 | 29.36 | |
| 3.004 | 45 | 3 0 1 + | 29.72 | |
| 2.934 | 2 | 3 1 1 | 30.44 | |
| 2.882 | 1 | 2 0 2 | 31.00 | |
| 2.820 | 6 | 2 1 2 + | 31.70 | |
| 2.751 | 1 | 3 2 1 | 32.52 | |
| 2.693 | 21 | 1 3 2 | 33.24 | |
| 2.623 | 2 | 2 4 1 | 34.16 | |
| 2.510 | 4 | 3 3 1 | 35.74 | |
| 2.439 | 4 | 2 3 2 | 36.82 | |
| 2.419 | 1 | 3 0 2 | 37.14 | |
| 2.385 | 1 | 3 4 0 | 37.68 | |
| 2.347 | 9 | 4 0 1 | 38.32 | |
| 2.287 | 25 | 0 6 0 | 39.36 | |
| 2.260 | 2 | 3 4 1 | 39.86 | |
| 2.220 | 1 | 4 2 1 | 40.60 | |
| 2.185 | 18 | 4 3 0 | 41.28 | |
| 2.179 | 11 | 1 2 3 | 41.40 | |
| 2.139 | 41 | 3 3 2 | 42.22 | |
| 2.132 | 27 | 2 0 3 | 42.36 | |
| 2.126 | 14 | 1 6 1 | 42.48 | |
| 2.105 | 2 | 2 1 3 | 42.92 | |
| 2.095 | 8 | 0 3 3 | 43.14 | |
| 2.088 | 9 | 4 3 1 | 43.30 | |
| 2.051 | 3 | 1 3 3 | 44.12 | |
| 2.034 | 2 | 2 2 3 | 44.50 | |
| 2.027 | 1 | 3 5 1 | 44.68 | |
| 1.994 | 8 | 2 6 1 | 45.44 | |
| 1.989 | 6 | 2 5 2 | 45.58 | |

Potassium zinc iodide hydrate, $\text{KZnI}_3 \cdot 2\text{H}_2\text{O}$ – continued

| $d (\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ $\lambda = 1.54056 \text{\AA}$ | Calculated Pattern (Integrated) | | | |
|------------------|-----|-------|---|---------------------------------|-----|-------|---|
| | | | | $d (\text{\AA})$ | I | hkl | $2\theta (\text{\\circ})$ $\lambda = 1.54056 \text{\AA}$ |
| 1.931 | 16 | 2 3 3 | 47.02 | 8.06 | 3 | 1 1 0 | 10.97 |
| 1.921 | 4 | 3 0 3 | + 47.28 | 6.86 | 8 | 0 2 0 | 12.89 |
| 1.916 | 5 | 5 0 1 | 47.42 | 6.29 | 5 | 0 1 1 | 14.08 |
| 1.886 | 19 | 1 6 2 | 48.22 | 5.76 | 52 | 1 0 1 | 15.36 |
| 1.859 | 1 | 4 3 2 | 48.96 | 5.65 | 5 | 1 2 0 | 15.67 |
| 1.857 | 1 | 1 7 1 | 49.02 | 5.31 | 7 | 1 1 1 | 16.67 |
| 1.845 | 1 | 5 2 1 | 49.36 | 4.975 | 5 | 2 0 0 | 17.81 |
| 1.820 | 12 | 3 6 1 | 50.08 | 4.925 | 12 | 0 2 1 | 18.00 |
| 1.815 | 7 | 3 5 2 | 50.22 | 4.414 | 2 | 1 2 1 | 20.10 |
| 1.810 | 2 | 2 4 3 | 50.36 | 4.069 | 45 | 2 0 1 | 21.82 |
| 1.784 | 1 | 4 5 1 | 51.16 | 3.901 | 3 | 2 1 1 | 22.78 |
| 1.767 | 20 | 5 3 1 | + 51.68 | 3.842 | 17 | 0 3 1 | 23.13 |
| 1.741 | 2 | 1 0 4 | 52.52 | 3.584 | 100 | 1 3 1 | 24.82 |
| 1.734 | 2 | 5 0 2 | 52.74 | 3.536 | 6 | 0 0 2 | 25.16 |
| 1.715 | 2 | 0 7 2 | 53.38 | 3.500 | 2 | 2 2 1 | 25.43 |
| 1.711 | 7 | 4 0 3 | 53.52 | 3.424 | 7 | 0 1 2 | 26.00 |
| 1.673 | 1 | 5 4 1 | 54.84 | 3.368 | 79 | 2 3 0 | 26.44 |
| 1.668 | 1 | 0 8 1 | 55.02 | 3.332 | 88 | 1 0 2 | 26.73 |
| 1.658 | 4 | 6 0 0 | 55.36 | 3.238 | 2 | 1 1 2 | 27.53 |
| 1.638 | 4 | 4 6 1 | 56.10 | 3.224 | 2 | 3 1 0 | 27.65 |
| 1.627 | 2 | 1 3 4 | 56.52 | 3.087 | 1 | 0 4 1 | 28.89 |
| 1.622 | 4 | 5 3 2 | + 56.72 | 3.041 | 49 | 2 3 1 | 29.35 |
| 1.602 | 4 | 4 3 3 | 57.46 | 3.003 | 49 | 3 0 1 | 29.73 |
| 1.574 | 1 | 3 5 3 | 58.60 | 2.997 | 1 | 1 2 2 | 29.78 |
| 1.565 | 5 | 2 3 4 | 58.96 | 2.933 | 1 | 3 1 1 | 30.45 |
| 1.559 | 6 | 2 6 3 | 59.22 | 2.882 | 1 | 2 0 2 | 31.00 |
| 1.548 | 1 | 5 4 2 | 59.68 | 2.825 | 2 | 2 4 0 | 31.65 |
| 1.523 | 3 | 6 3 1 | 60.78 | 2.821 | 5 | 2 1 2 | 31.70 |
| 1.476 | 2 | 3 3 4 | 62.90 | 2.751 | 1 | 3 2 1 | 32.52 |
| 1.475 | 3 | 1 9 1 | 62.98 | 2.693 | 22 | 1 3 2 | 33.24 |
| 1.471 | 3 | 3 6 3 | 63.16 | 2.623 | 2 | 2 4 1 | 34.15 |
| 1.469 | 2 | 5 6 1 | 63.26 | 2.511 | 4 | 3 3 1 | 35.74 |
| 1.458 | 2 | 2 9 0 | 63.78 | 2.439 | 5 | 2 3 2 | 36.83 |
| 1.443 | 2 | 5 3 3 | 64.52 | 2.419 | 1 | 3 0 2 | 37.13 |
| 1.428 | 2 | 2 9 1 | 65.28 | 2.385 | 1 | 3 4 0 | 37.69 |
| 1.399 | 4 | 0 6 4 | + 66.82 | 2.347 | 10 | 4 0 1 | 38.33 |
| 1.386 | 1 | 1 9 2 | 67.50 | 2.294 | 2 | 1 0 3 | 39.24 |
| 1.385 | 2 | 1 6 4 | 67.56 | 2.288 | 29 | 0 6 0 | 39.35 |
| 1.382 | 2 | 5 6 2 | 67.74 | 2.276 | 1 | 2 5 1 | 39.57 |
| 1.375 | 4 | 4 3 4 | 68.16 | 2.260 | 1 | 3 4 1 | 39.86 |
| 1.370 | 5 | 4 6 3 | 68.40 | 2.220 | 1 | 4 2 1 | 40.60 |
| 1.3426 | 3 | 6 6 0 | 70.02 | 2.185 | 21 | 4 3 0 | 41.28 |
| 1.3393 | 4 | 1 3 5 | 70.22 | 2.176 | 1 | 1 2 3 | 41.47 |
| 1.3330 | 1 | 7 3 1 | 70.60 | 2.139 | 48 | 3 3 2 | 42.22 |
| 1.3187 | 3 | 7 0 2 | 71.48 | 2.130 | 14 | 2 0 3 | 42.40 |
| 1.3005 | 5 | 6 3 3 | + 72.64 | 2.126 | 7 | 1 6 1 | 42.47 |
| 1.2901 | 3 | 3 9 2 | 73.32 | 2.105 | 1 | 2 1 3 | 42.93 |
| 1.2805 | 1 | 0 9 3 | 73.96 | 2.096 | 9 | 0 3 3 | 43.13 |
| 1.2787 | 1 | 4 9 1 | 74.08 | 2.088 | 8 | 4 3 1 | 43.30 |
| 1.2401 | 2 | 2 9 3 | 76.80 | 2.051 | 3 | 1 3 3 | 44.13 |

Potassium zinc iodide hydrate, KZnI₃·2H₂O – continued

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2θ(°) λ = 1.54056 Å |
|--------------|----------|------------|------------------------|
| 2.035 | 2 | 2 2 3 | 44.49 |
| 2.026 | 1 | 3 5 1 | 44.69 |
| 1.994 | 9 | 2 6 1 | 45.44 |
| 1.988 | 3 | 2 5 2 | 45.60 |
| 1.937 | 1 | 4 4 1 | 46.86 |
| 1.931 | 19 | 2 3 3 | 47.01 |
| 1.921 | 2 | 3 0 3 | 47.27 |
| 1.921 | 1 | 0 6 2 | 47.28 |
| 1.916 | 4 | 5 0 1 | 47.42 |
| 1.890 | 1 | 0 7 1 | 48.11 |
| 1.886 | 25 | 1 6 2 | 48.21 |
| 1.859 | 1 | 4 3 2 | 48.96 |
| 1.857 | 1 | 1 7 1 | 49.03 |
| 1.845 | 1 | 5 2 1 | 49.35 |
| 1.820 | 15 | 3 6 1 | 50.08 |
| 1.815 | 1 | 3 5 2 | 50.22 |
| 1.810 | 2 | 2 4 3 | 50.38 |
| 1.784 | 1 | 4 5 1 | 51.17 |
| 1.768 | 9 | 0 0 4 | 51.66 |
| 1.767 | 18 | 5 3 1 | 51.69 |
| 1.741 | 2 | 1 0 4 | 52.53 |
| 1.734 | 2 | 5 0 2 | 52.74 |
| 1.715 | 1 | 0 7 2 | 53.38 |
| 1.711 | 8 | 4 0 3 | 53.51 |
| 1.673 | 1 | 5 4 1 | 54.84 |
| 1.667 | 1 | 0 8 1 | 55.02 |
| 1.658 | 5 | 6 0 0 | 55.35 |
| 1.638 | 4 | 4 6 1 | 56.10 |
| 1.627 | 2 | 1 3 4 | 56.52 |
| 1.622 | 4 | 5 3 2 | 56.72 |
| 1.620 | 1 | 1 6 3 | 56.79 |
| 1.603 | 5 | 4 3 3 | 57.45 |
| 1.574 | 1 | 3 5 3 | 58.59 |
| 1.565 | 7 | 2 3 4 | 58.95 |
| 1.559 | 8 | 2 6 3 | 59.22 |
| 1.548 | 1 | 5 4 2 | 59.69 |
| 1.523 | 3 | 6 3 1 | 60.78 |
| 1.477 | 2 | 3 3 4 | 62.88 |
| 1.474 | 4 | 1 9 1 | 62.99 |
| 1.471 | 1 | 3 6 3 | 63.14 |
| 1.469 | 3 | 5 6 1 | 63.26 |
| 1.458 | 3 | 2 9 0 | 63.77 |
| 1.443 | 2 | 5 3 3 | 64.52 |
| 1.428 | 3 | 2 9 1 | 65.28 |
| 1.400 | 1 | 1 0 5 | 66.74 |
| 1.399 | 6 | 0 6 4 | 66.82 |
| 1.387 | 1 | 1 9 2 | 67.48 |
| 1.385 | 2 | 1 6 4 | 67.56 |
| 1.382 | 2 | 5 6 2 | 67.75 |
| 1.375 | 5 | 4 3 4 | 68.17 |

| <i>d</i> (Å) | <i>I</i> | <i>hkl</i> | 2θ(°) λ = 1.54056 Å |
|--------------|----------|------------|------------------------|
| 1.370 | 5 | 4 6 3 | 68.41 |
| 1.3427 | 4 | 6 6 0 | 70.01 |
| 1.3390 | 4 | 1 3 5 | 70.24 |
| 1.3331 | 1 | 7 3 1 | 70.59 |
| 1.3189 | 5 | 7 0 2 | 71.47 |
| 1.3010 | 3 | 3 0 5 | 72.61 |
| 1.3004 | 4 | 6 3 3 | 72.65 |
| 1.3003 | 2 | 4 9 0 | 72.66 |
| 1.2902 | 5 | 3 9 2 | 73.32 |
| 1.2806 | 1 | 0 9 3 | 73.96 |
| 1.2788 | 1 | 4 9 1 | 74.07 |
| 1.2401 | 2 | 2 9 3 | 76.80 |
| 1.2095 | 2 | 6 0 4 | 79.11 |
| 1.2002 | 1 | 8 3 0 | 79.85 |
| 1.1944 | 1 | 1 6 5 | 80.32 |
| 1.1932 | 3 | 5 9 1 | 80.41 |

Sodium D-tartrate hydrate, $(\text{CHOH-CO}_2\text{Na})_2 \cdot 2\text{H}_2\text{O}$

Structure

Orthorhombic, $P2_12_12_1$ (19), $Z=4$. The structure was determined by Ambady and Kartha [1968].

Lattice parameters

$a=11.460(5)$, $b=14.670(5)$, $c=4.959(3)\text{\AA}$ [ibid.]

Density

(calculated) 1.833 g/cm^3

Thermal parameters

Anisotropic [ibid.]

Scattering factors

H^0 , C^0 , O^0 , Na^+ [International Tables, 1962]

Scale factors

(integrated intensities) 2.400×10^4

Reference

Ambady, G.K. and Kartha, G. (1968). Acta Cryst. B24, 1540.

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

| $d (\text{\AA})$ | I | hkl | $2\theta (\text{^\circ})$ | $\lambda = 1.54056 \text{\AA}$ |
|------------------|-----|---------|---------------------------|--------------------------------|
| 3.482 | 22 | 0 3 1 | 25.56 | |
| 3.388 | 4 | 3 2 0 | 26.28 | |
| 3.331 | 22 | 1 3 1 + | 26.74 | |
| 3.089 | 1 | 2 4 0 | 28.88 | |
| 3.009 | 2 | 3 3 0 | 29.66 | |
| 2.965 | 18 | 3 1 1 | 30.12 | |
| 2.864 | 20 | 4 0 0 | 31.20 | |
| 2.857 | 25 | 1 4 1 | 31.28 | |
| 2.798 | 49 | 3 2 1 | 31.96 | |
| 2.668 | 8 | 4 2 0 | 33.56 | |
| 2.645 | 4 | 3 4 0 | 33.86 | |
| 2.621 | 14 | 2 4 1 | 34.18 | |
| 2.614 | 11 | 2 5 0 | 34.28 | |
| 2.573 | 8 | 3 3 1 | 34.84 | |
| 2.525 | 2 | 0 5 1 | 35.52 | |
| 2.481 | 28 | 4 0 1 + | 36.18 | |
| 2.473 | 18 | 4 3 0 | 36.30 | |
| 2.466 | 12 | 1 5 1 | 36.40 | |
| 2.445 | 5 | 4 1 1 + | 36.72 | |
| 2.424 | 4 | 1 0 2 | 37.06 | |
| 2.391 | 4 | 1 6 0 | 37.58 | |
| 2.349 | 5 | 4 2 1 + | 38.28 | |
| 2.334 | 1 | 3 4 1 | 38.54 | |
| 2.327 | 3 | 3 5 0 | 38.66 | |
| 2.311 | 22 | 2 5 1 | 38.94 | |
| 2.304 | 13 | 1 2 2 | 39.06 | |
| 2.264 | 1 | 5 1 0 | 39.78 | |
| 2.258 | 3 | 4 4 0 | 39.90 | |
| 2.249 | 6 | 2 6 0 | 40.06 | |
| 2.212 | 1 | 0 3 2 | 40.76 | |
| 2.187 | 3 | 5 2 0 | 41.24 | |
| 2.173 | 5 | 2 2 2 + | 41.52 | |
| 2.154 | 9 | 1 6 1 | 41.90 | |
| 2.106 | 1 | 3 5 1 | 42.90 | |
| 2.080 | 1 | 3 0 2 | 43.48 | |
| 2.062 | 10 | 2 3 2 + | 43.88 | |
| 2.054 | 11 | 4 4 1 + | 44.04 | |
| 2.050 | 6 | 4 5 0 | 44.14 | |
| 2.022 | 1 | 1 4 2 | 44.78 | |
| 2.001 | 4 | 5 2 1 + | 45.28 | |
| 1.968 | 2 | 2 7 0 | 46.08 | |
| 1.933 | 2 | 2 4 2 | 46.96 | |
| 1.930 | 2 | 0 7 1 | 47.04 | |
| 1.914 | 4 | 3 3 2 | 47.46 | |
| 1.904 | 3 | 1 7 1 | 47.74 | |
| 1.894 | 4 | 6 1 0 + | 48.00 | |
| 1.860 | 8 | 4 1 2 + | 48.94 | |

| Calculated Pattern (Peak heights) | | | | |
|-----------------------------------|-----|-------|---------------------------|--------------------------------|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{^\circ})$ | $\lambda = 1.54056 \text{\AA}$ |
| 9.02 | 100 | 1 1 0 | 9.80 | |
| 6.171 | 10 | 1 2 0 | 14.34 | |
| 5.727 | 29 | 2 0 0 | 15.46 | |
| 4.696 | 25 | 0 1 1 | 18.88 | |
| 4.548 | 14 | 1 0 1 | 19.50 | |
| 4.498 | 22 | 1 3 0 | 19.72 | |
| 3.867 | 6 | 1 2 1 | 22.98 | |
| 3.720 | 2 | 2 3 0 | 23.90 | |
| 3.666 | 4 | 0 4 0 | 24.26 | |
| 3.633 | 35 | 2 1 1 | 24.48 | |

Sodium D-tartrate hydrate, $(\text{CHOH-CO}_2\text{Na})_2 \cdot 2\text{H}_2\text{O}$ – continued

| d (Å) | I | hkl | $2\theta (\circ)$ $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|---------|--|
| 1.848 | 3 | 6 2 0 | 49.26 |
| 1.837 | 1 | 3 7 0 | 49.58 |
| 1.829 | 3 | 2 7 1 | 49.80 |
| 1.817 | 4 | 4 2 2 | 50.18 |
| 1.810 | 3 | 5 4 1 | 50.38 |
| 1.806 | 2 | 5 5 0 | 50.50 |
| 1.798 | 7 | 2 5 2 | 50.72 |
| 1.779 | 2 | 6 3 0 | 51.32 |
| 1.769 | 1 | 6 1 1 | 51.62 |
| 1.750 | 1 | 4 3 2 | 52.22 |
| 1.747 | 2 | 2 8 0 | 52.34 |
| 1.742 | 2 | 4 6 1 | 52.50 |
| 1.732 | 1 | 6 2 1 | 52.82 |
| 1.721 | 2 | 1 6 2 | 53.16 |
| 1.701 | 1 | 1 8 1 | 53.86 |
| 1.697 | 3 | 5 5 1 + | 54.00 |
| 1.694 | 4 | 6 4 0 | 54.10 |
| 1.647 | 2 | 2 8 1 | 55.76 |
| 1.636 | 1 | 1 0 3 | 56.16 |
| 1.626 | 1 | 1 1 3 | 56.56 |
| 1.600 | 1 | 6 5 0 + | 57.54 |
| 1.597 | 3 | 1 2 3 + | 57.68 |
| 1.592 | 2 | 5 3 2 | 57.88 |
| 1.584 | 3 | 5 6 1 + | 58.18 |
| 1.580 | 2 | 2 1 3 | 58.36 |
| 1.568 | 2 | 3 8 1 | 58.84 |
| 1.555 | 2 | 7 0 1 | 59.40 |
| 1.551 | 3 | 1 3 3 | 59.54 |
| 1.547 | 2 | 7 1 1 + | 59.72 |
| 1.542 | 1 | 2 7 2 | 59.94 |
| 1.517 | 1 | 3 0 3 | 61.02 |
| 1.513 | 1 | 6 0 2 | 61.20 |
| 1.511 | 3 | 2 3 3 + | 61.32 |
| 1.505 | 2 | 6 1 2 | 61.56 |
| 1.495 | 1 | 7 4 0 | 62.04 |
| 1.488 | 1 | 4 6 2 | 62.36 |
| 1.486 | 1 | 3 2 3 | 62.46 |
| 1.482 | 2 | 7 3 1 + | 62.64 |
| 1.477 | 1 | 5 7 1 | 62.88 |
| 1.467 | 1 | 0 10 0 | 63.34 |
| 1.432 | 1 | 7 4 1 + | 65.10 |
| 1.428 | 2 | 2 8 2 + | 65.28 |
| 1.417 | 1 | 4 9 0 | 65.86 |
| 1.412 | 1 | 6 7 0 | 66.14 |
| 1.370 | 1 | 8 1 1 | 68.42 |
| 1.227 | 1 | 6 7 2 | 77.78 |
| 1.222 | 1 | 0 2 4 | 78.12 |
| 1.220 | 1 | 5 5 3 | 78.34 |
| 1.175 | 1 | 0 11 2 | 81.96 |

| Calculated Pattern (Integrated) | | | |
|---------------------------------|-----|-------|--|
| d (Å) | I | hkl | $2\theta (\circ)$ $\lambda = 1.54056 \text{ Å}$ |
| 9.03 | 100 | 1 1 0 | 9.79 |
| 6.178 | 11 | 1 2 0 | 14.32 |
| 5.730 | 32 | 2 0 0 | 15.45 |
| 4.698 | 28 | 0 1 1 | 18.87 |
| 4.551 | 15 | 1 0 1 | 19.49 |
| 4.516 | 4 | 2 2 0 | 19.64 |
| 4.498 | 24 | 1 3 0 | 19.72 |
| 3.867 | 7 | 1 2 1 | 22.98 |
| 3.720 | 2 | 2 3 0 | 23.90 |
| 3.667 | 4 | 0 4 0 | 24.25 |
| 3.633 | 44 | 2 1 1 | 24.48 |
| 3.482 | 27 | 0 3 1 | 25.56 |
| 3.388 | 5 | 3 2 0 | 26.28 |
| 3.339 | 13 | 2 2 1 | 26.68 |
| 3.332 | 19 | 1 3 1 | 26.74 |
| 3.089 | 1 | 2 4 0 | 28.88 |
| 3.010 | 2 | 3 3 0 | 29.65 |
| 2.964 | 25 | 3 1 1 | 30.13 |
| 2.865 | 24 | 4 0 0 | 31.19 |
| 2.856 | 24 | 1 4 1 | 31.30 |
| 2.797 | 68 | 3 2 1 | 31.97 |
| 2.669 | 11 | 4 2 0 | 33.55 |
| 2.646 | 5 | 3 4 0 | 33.85 |
| 2.622 | 20 | 2 4 1 | 34.17 |
| 2.612 | 8 | 2 5 0 | 34.31 |
| 2.573 | 11 | 3 3 1 | 34.84 |
| 2.525 | 2 | 0 5 1 | 35.52 |
| 2.481 | 36 | 4 0 1 | 36.18 |
| 2.479 | 3 | 0 0 2 | 36.20 |
| 2.472 | 5 | 4 3 0 | 36.31 |
| 2.466 | 11 | 1 5 1 | 36.40 |
| 2.446 | 4 | 4 1 1 | 36.71 |
| 2.445 | 2 | 0 6 0 | 36.73 |
| 2.423 | 5 | 1 0 2 | 37.07 |
| 2.391 | 6 | 1 6 0 | 37.58 |
| 2.350 | 7 | 4 2 1 | 38.27 |
| 2.349 | 1 | 0 2 2 | 38.29 |
| 2.334 | 1 | 3 4 1 | 38.54 |
| 2.327 | 3 | 3 5 0 | 38.66 |
| 2.311 | 32 | 2 5 1 | 38.94 |
| 2.301 | 2 | 1 2 2 | 39.11 |
| 2.265 | 1 | 5 1 0 | 39.77 |
| 2.258 | 4 | 4 4 0 | 39.90 |
| 2.249 | 7 | 2 6 0 | 40.06 |
| 2.211 | 1 | 0 3 2 | 40.77 |
| 2.193 | 1 | 0 6 1 | 41.13 |
| 2.188 | 4 | 5 2 0 | 41.23 |
| 2.173 | 6 | 2 2 2 | 41.51 |
| 2.171 | 3 | 1 3 2 | 41.55 |
| 2.154 | 13 | 1 6 1 | 41.91 |

Sodium D-tartrate hydrate, $(\text{CHOH-CO}_2\text{Na})_2 \cdot 2\text{H}_2\text{O}$ – continued

| d (Å) | I | hkl | $2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$ | d (Å) | I | hkl | $2\theta(^{\circ})$ $\lambda = 1.54056 \text{ Å}$ |
|---------|-----|-------|--|---------|-----|--------|--|
| 2.106 | 1 | 3 5 1 | 42.90 | 1.579 | 1 | 2 1 3 | 58.40 |
| 2.080 | 1 | 3 0 2 | 43.48 | 1.568 | 2 | 3 8 1 | 58.83 |
| 2.063 | 8 | 2 3 2 | 43.85 | 1.555 | 3 | 7 0 1 | 59.40 |
| 2.062 | 7 | 1 7 0 | 43.88 | 1.552 | 4 | 1 3 3 | 59.53 |
| 2.060 | 2 | 5 1 1 | 43.92 | 1.548 | 1 | 0 9 1 | 59.66 |
| 2.059 | 2 | 3 1 2 | 43.93 | 1.547 | 1 | 5 7 0 | 59.74 |
| 2.055 | 8 | 4 4 1 | 44.03 | 1.546 | 1 | 7 1 1 | 59.77 |
| 2.054 | 3 | 0 4 2 | 44.05 | 1.542 | 1 | 2 7 2 | 59.96 |
| 2.050 | 2 | 4 5 0 | 44.14 | 1.523 | 1 | 6 5 1 | 60.75 |
| 2.022 | 2 | 1 4 2 | 44.79 | 1.517 | 1 | 3 0 3 | 61.03 |
| 2.002 | 3 | 5 2 1 | 45.27 | 1.513 | 1 | 6 0 2 | 61.20 |
| 2.001 | 3 | 3 2 2 | 45.28 | 1.511 | 4 | 2 3 3 | 61.32 |
| 1.968 | 3 | 2 7 0 | 46.08 | 1.509 | 1 | 3 1 3 | 61.39 |
| 1.934 | 3 | 2 4 2 | 46.95 | 1.505 | 1 | 6 1 2 | 61.56 |
| 1.930 | 2 | 0 7 1 | 47.03 | 1.495 | 2 | 7 4 0 | 62.03 |
| 1.914 | 6 | 3 3 2 | 47.47 | 1.488 | 2 | 4 6 2 | 62.36 |
| 1.904 | 4 | 1 7 1 | 47.74 | 1.486 | 1 | 3 2 3 | 62.46 |
| 1.894 | 5 | 6 1 0 | 47.99 | 1.482 | 1 | 6 2 2 | 62.64 |
| 1.894 | 1 | 0 5 2 | 48.00 | 1.482 | 1 | 7 3 1 | 62.65 |
| 1.860 | 2 | 4 6 0 | 48.93 | 1.476 | 1 | 5 7 1 | 62.89 |
| 1.860 | 11 | 4 1 2 | 48.94 | 1.467 | 2 | 0 10 0 | 63.35 |
| 1.848 | 4 | 6 2 0 | 49.26 | 1.460 | 1 | 5 5 2 | 63.69 |
| 1.837 | 1 | 3 7 0 | 49.57 | 1.432 | 1 | 5 8 0 | 65.09 |
| 1.829 | 4 | 2 7 1 | 49.80 | 1.431 | 1 | 7 4 1 | 65.12 |
| 1.816 | 7 | 4 2 2 | 50.18 | 1.430 | 1 | 7 5 0 | 65.20 |
| 1.810 | 3 | 5 4 1 | 50.38 | 1.429 | 1 | 1 5 3 | 65.24 |
| 1.806 | 1 | 5 5 0 | 50.49 | 1.428 | 1 | 2 8 2 | 65.30 |
| 1.798 | 12 | 2 5 2 | 50.73 | 1.417 | 1 | 4 9 0 | 65.87 |
| 1.779 | 3 | 6 3 0 | 51.31 | 1.412 | 1 | 6 7 0 | 66.14 |
| 1.769 | 2 | 6 1 1 | 51.61 | 1.370 | 1 | 8 1 1 | 68.41 |
| 1.751 | 1 | 4 3 2 | 52.21 | 1.362 | 1 | 0 9 2 | 68.88 |
| 1.746 | 3 | 2 8 0 | 52.34 | 1.353 | 1 | 8 2 1 | 69.43 |
| 1.741 | 2 | 4 6 1 | 52.51 | 1.348 | 1 | 3 5 3 | 69.72 |
| 1.732 | 1 | 6 2 1 | 52.81 | 1.227 | 1 | 6 7 2 | 77.79 |
| 1.721 | 3 | 1 6 2 | 53.17 | 1.222 | 1 | 0 2 4 | 78.12 |
| 1.701 | 1 | 1 8 1 | 53.86 | 1.219 | 1 | 5 5 3 | 78.35 |
| 1.697 | 2 | 5 5 1 | 53.98 | 1.175 | 1 | 0 11 2 | 81.96 |
| 1.697 | 2 | 3 5 2 | 54.00 | | | | |
| 1.694 | 5 | 6 4 0 | 54.09 | | | | |
| 1.675 | 1 | 6 3 1 | 54.77 | | | | |
| 1.647 | 4 | 2 8 1 | 55.76 | | | | |
| 1.636 | 1 | 1 0 3 | 56.17 | | | | |
| 1.626 | 2 | 1 1 3 | 56.55 | | | | |
| 1.601 | 1 | 4 7 1 | 57.52 | | | | |
| 1.601 | 1 | 6 5 0 | 57.53 | | | | |
| 1.598 | 2 | 7 2 0 | 57.64 | | | | |
| 1.597 | 3 | 1 2 3 | 57.68 | | | | |
| 1.591 | 2 | 5 3 2 | 57.90 | | | | |
| 1.585 | 2 | 5 6 1 | 58.17 | | | | |
| 1.584 | 2 | 3 6 2 | 58.19 | | | | |

Yttrium titanium oxide, Y_2TiO_5

Structure

Orthorhombic, Pnam (62), Z=4. The structure was determined by Mumme and Wadsley (1968).

Lattice parameters

$a=10.35(1)$, $b=11.25(1)$, $c=3.70(1)\text{\AA}$ [ibid.]

Density
(calculated) 4.713 g/cm^3

Thermal parameters

Isotropic [ibid.]

Scattering factors

O^{2-} [Suzuki, 1960]

Y^{3+} , Ti^{4+} [Cromer and Waber, 1965]. These factors were corrected for dispersion [Cromer, 1965].

Scale factors

(integrated intensities) 10.05×10^4

Additional patterns

1. PDF card 21-1464 [Garton and Wanklyn, 1968]

Reference

- Cromer, D.T. (1965). Acta Cryst. **18**, 17.
- Cromer, D.T. and Waber, J.T. (1965). Acta Cryst. **18**, 104.
- Garton, G. and Wanklyn, B.M. (1968). J. Mater.Sci. **3**, 395.
- Mumme, W.G. and Wadsley, A.D. (1968). Acta Cryst. **B24**, 1327.
- Suzuki, T. (1960). Acta Cryst. **13**, 279.

| Calculated Pattern (Peak heights) | | | |
|-----------------------------------|-----|---------|---|
| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ $\lambda = 1.54056 \text{\AA}$ |
| 7.61 | 18 | 1 1 0 | 11.62 |
| 5.63 | 2 | 0 2 0 | 15.74 |
| 5.18 | 11 | 2 0 0 | 17.12 |
| 4.94 | 3 | 1 2 0 | 17.94 |
| 4.70 | 6 | 2 1 0 | 18.86 |
| 3.81 | 2 | 2 2 0 | 23.34 |
| 3.53 | 24 | 1 3 0 + | 25.24 |
| 3.33 | 2 | 1 1 1 | 26.76 |
| 3.04 | 74 | 2 3 0 | 29.40 |
| 3.01 | 100 | 2 0 1 | 29.66 |

| $d (\text{\AA})$ | I | hkl | $2\theta (\text{)}^\circ$ $\lambda = 1.54056 \text{\AA}$ |
|------------------|-----|---------|---|
| 2.94 | 9 | 3 2 0 | 30.36 |
| 2.91 | 4 | 2 1 1 | 30.72 |
| 2.71 | 2 | 1 4 0 | 32.98 |
| 2.63 | 25 | 0 3 1 | 34.02 |
| 2.587 | 8 | 4 0 0 | 34.64 |
| 2.552 | 9 | 1 3 1 | 35.14 |
| 2.539 | 8 | 3 3 0 | 35.32 |
| 2.521 | 4 | 4 1 0 | 35.58 |
| 2.462 | 3 | 3 1 1 | 36.46 |
| 2.302 | 7 | 3 2 1 | 39.10 |
| 2.198 | 4 | 1 5 0 | 41.02 |
| 2.130 | 1 | 4 3 0 | 42.40 |
| 2.121 | 2 | 4 0 1 | 42.60 |
| 2.093 | 8 | 3 3 1 | 43.18 |
| 2.084 | 4 | 4 1 1 | 43.38 |
| 2.055 | 3 | 2 4 1 | 44.02 |
| 2.036 | 2 | 5 1 0 | 44.46 |
| 1.984 | 3 | 4 2 1 | 45.68 |
| 1.943 | 1 | 5 2 0 | 46.72 |
| 1.904 | 3 | 4 4 0 | 47.72 |
| 1.890 | 1 | 1 5 1 | 48.10 |
| 1.875 | 4 | 0 6 0 | 48.52 |
| 1.850 | 23 | 0 0 2 | 49.22 |
| 1.845 | 55 | 4 3 1 + | 49.34 |
| 1.798 | 1 | 1 1 2 | 50.74 |
| 1.783 | 2 | 5 1 1 | 51.18 |
| 1.720 | 6 | 5 2 1 | 53.20 |
| 1.705 | 1 | 6 1 0 | 53.72 |
| 1.693 | 1 | 4 4 1 | 54.12 |
| 1.679 | 2 | 3 5 1 | 54.60 |
| 1.667 | 1 | 5 4 0 | 55.04 |
| 1.651 | 10 | 1 6 1 + | 55.62 |
| 1.647 | 7 | 3 6 0 | 55.76 |
| 1.638 | 4 | 1 3 2 | 56.10 |
| 1.627 | 4 | 5 3 1 | 56.50 |
| 1.591 | 5 | 2 6 1 | 57.90 |
| 1.580 | 15 | 2 3 2 | 58.36 |
| 1.567 | 5 | 6 3 0 + | 58.88 |
| 1.563 | 7 | 6 0 1 | 59.04 |
| 1.549 | 2 | 6 1 1 | 59.66 |
| 1.524 | 1 | 5 5 0 | 60.74 |
| 1.519 | 2 | 4 6 0 | 60.96 |
| 1.505 | 10 | 3 6 1 + | 61.58 |
| 1.495 | 2 | 3 3 2 | 62.02 |
| 1.492 | 2 | 4 1 2 | 62.18 |
| 1.470 | 1 | 6 4 0 | 63.18 |
| 1.466 | 2 | 7 1 0 | 63.38 |
| 1.443 | 1 | 6 3 1 | 64.52 |
| 1.430 | 1 | 7 2 0 | 65.18 |
| 1.418 | 1 | 2 7 1 | 65.82 |
| 1.415 | 1 | 1 5 2 | 65.94 |

Yttrium titanium oxide, Y_2TiO_5 – continued

| d (\AA) | I | hkl | 2θ ($^\circ$) | $\lambda = 1.54056 \text{\AA}$ |
|----------------------|-----|--------|------------------------|--------------------------------|
| | | | $^\circ$ | |
| 1.390 | 2 | 5 6 0 | 67.32 | |
| 1.369 | 1 | 5 1 2 | 68.48 | |
| 1.367 | 2 | 6 4 1 | 68.62 | |
| 1.363 | 1 | 7 1 1 | 68.82 | |
| 1.327 | 1 | 4 4 2 | 70.98 | |
| 1.317 | 1 | 0 6 2 | 71.60 | |
| 1.306 | 6 | 1 6 2 | 72.26 | |
| 1.294 | 1 | 8 0 0 | 73.08 | |
| 1.285 | 1 | 8 1 0 | 73.64 | |
| 1.281 | 1 | 4 7 1 | 73.94 | |
| 1.241 | 1 | 1 9 0 | 76.74 | |
| 1.234 | 1 | 7 4 1 | 77.26 | |
| 1.230 | 1 | 3 6 2 | 77.52 | |
| 1.200 | 4 | 2 0 3 | 79.88 | |
| 1.196 | 3 | 6 3 2 | 80.20 | |
| 1.193 | 2 | 8 2 1 | 80.44 | |
| 1.176 | 4 | 1 9 1 | 81.88 | |
| 1.174 | 4 | 4 6 2 | 82.04 | |
| 1.172 | 4 | 0 3 3 | 82.20 | |
| 1.164 | 1 | 1 3 3 | 82.86 | |
| 1.161 | 1 | 8 3 1 | 83.12 | |
| 1.151 | 1 | 6 4 2 | 84.00 | |
| 1.149 | 1 | 7 1 2 | 84.20 | |
| 1.131 | 1 | 7 2 2 | 85.82 | |
| 1.120 | 2 | 3 9 1 | 86.90 | |
| 1.111 | 2 | 5 6 2 | 87.78 | |
| 1.109 | 2 | 5 8 1 | 87.94 | |
| 1.108 | 2 | 7 6 1 | 88.10 | |
| 1.104 | 1 | 7 3 2 | 88.50 | |
| 1.093 | 1 | 9 1 1 | 89.62 | |
| 1.070 | 1 | 5 9 0 | 92.08 | |
| 1.067 | 3 | 4 3 3 | 92.40 | |
| 1.060 | 1 | 8 0 2 | 93.20 | |
| 1.055 | 1 | 8 1 2 | 93.74 | |
| 1.044 | 1 | 7 7 1 | 95.10 | |
| 1.041 | 1 | 5 2 3 | 95.42 | |
| 1.031 | 2 | 1 9 2 | 96.74 | |
| 1.028 | 3 | 5 9 1 | 97.08 | |
| 1.025 | 3 | 1 6 3 | 97.40 | |
| 1.020 | 1 | 5 3 3 | 98.14 | |
| 1.011 | 1 | 2 6 3 | 99.32 | |
| 1.003 | 1 | 6 0 3 | 100.30 | |
| .992 | 3 | 3 9 2 | 101.88 | |
| .987 | 2 | 3 6 3 | 102.56 | |
| .972 | 1 | 8 7 1 | 104.78 | |
| .939 | 1 | 10 4 1 | 110.16 | |
| .934 | 1 | 1 12 0 | 111.18 | |
| .926 | 1 | 5 9 2 | 112.54 | |
| .925 | 1 | 0 0 4 | 112.76 | |
| .923 | 2 | 8 6 2 | 113.20 | |
| .911 | 1 | 10 5 1 | 115.40 | |

| Calculated Pattern (Integrated) | | | | |
|---------------------------------|-----|-------|------------------------|--------------------------------|
| d (\AA) | I | hkl | 2θ ($^\circ$) | $\lambda = 1.54056 \text{\AA}$ |
| 7.62 | 14 | 1 1 0 | 11.61 | |
| 5.63 | 2 | 0 2 0 | 15.74 | |
| 5.18 | 10 | 2 0 0 | 17.12 | |
| 4.94 | 2 | 1 2 0 | 17.93 | |
| 4.70 | 5 | 2 1 0 | 18.86 | |
| 3.81 | 2 | 2 2 0 | 23.34 | |
| 3.53 | 24 | 1 3 0 | 25.24 | |
| 3.51 | 1 | 0 1 1 | 25.32 | |
| 3.33 | 2 | 1 1 1 | 26.76 | |
| 3.04 | 78 | 2 3 0 | 29.39 | |
| 3.01 | 100 | 2 0 1 | 29.66 | |
| 2.94 | 9 | 3 2 0 | 30.37 | |
| 2.91 | 4 | 2 1 1 | 30.72 | |
| 2.71 | 2 | 1 4 0 | 32.98 | |
| 2.63 | 27 | 0 3 1 | 34.01 | |
| 2.588 | 8 | 4 0 0 | 34.64 | |
| 2.552 | 10 | 1 3 1 | 35.13 | |
| 2.539 | 8 | 3 3 0 | 35.32 | |
| 2.522 | 4 | 4 1 0 | 35.57 | |
| 2.462 | 3 | 3 1 1 | 36.46 | |
| 2.302 | 8 | 3 2 1 | 39.09 | |
| 2.199 | 4 | 1 5 0 | 41.02 | |
| 2.188 | 1 | 1 4 1 | 41.22 | |
| 2.130 | 1 | 4 3 0 | 42.41 | |
| 2.120 | 2 | 4 0 1 | 42.60 | |
| 2.093 | 9 | 3 3 1 | 43.18 | |
| 2.084 | 4 | 4 1 1 | 43.39 | |
| 2.055 | 3 | 2 4 1 | 44.03 | |
| 2.036 | 2 | 5 1 0 | 44.46 | |
| 1.984 | 4 | 4 2 1 | 45.69 | |
| 1.943 | 1 | 5 2 0 | 46.72 | |
| 1.904 | 3 | 4 4 0 | 47.72 | |
| 1.890 | 1 | 1 5 1 | 48.10 | |
| 1.878 | 2 | 3 4 1 | 48.42 | |
| 1.875 | 4 | 0 6 0 | 48.51 | |
| 1.850 | 22 | 0 0 2 | 49.21 | |
| 1.846 | 43 | 4 3 1 | 49.33 | |
| 1.845 | 16 | 1 6 0 | 49.35 | |
| 1.798 | 1 | 1 1 2 | 50.74 | |
| 1.784 | 2 | 5 1 1 | 51.17 | |
| 1.720 | 7 | 5 2 1 | 53.21 | |
| 1.705 | 2 | 6 1 0 | 53.71 | |
| 1.693 | 2 | 4 4 1 | 54.12 | |
| 1.679 | 3 | 3 5 1 | 54.60 | |
| 1.667 | 1 | 5 4 0 | 55.04 | |
| 1.651 | 13 | 1 6 1 | 55.62 | |
| 1.649 | 1 | 6 2 0 | 55.69 | |
| 1.647 | 1 | 3 6 0 | 55.75 | |
| 1.638 | 4 | 1 3 2 | 56.10 | |
| 1.627 | 5 | 5 3 1 | 56.50 | |

Yttrium titanium oxide, Y_2TiO_5 – continued

| d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ |
|----------------------|-----|-------|--|
| 1.591 | 6 | 2 6 1 | 57.90 |
| 1.580 | 20 | 2 3 2 | 58.36 |
| 1.567 | 5 | 6 3 0 | 58.88 |
| 1.566 | 2 | 3 2 2 | 58.93 |
| 1.563 | 7 | 6 0 1 | 59.03 |
| 1.549 | 3 | 6 1 1 | 59.66 |
| 1.523 | 2 | 5 5 0 | 60.75 |
| 1.518 | 2 | 4 6 0 | 60.97 |
| 1.505 | 9 | 3 6 1 | 61.57 |
| 1.505 | 4 | 4 0 2 | 61.57 |
| 1.495 | 3 | 3 3 2 | 62.02 |
| 1.492 | 1 | 4 1 2 | 62.18 |
| 1.474 | 1 | 0 7 1 | 63.01 |
| 1.470 | 2 | 6 4 0 | 63.18 |
| 1.466 | 2 | 7 1 0 | 63.40 |
| 1.443 | 1 | 6 3 1 | 64.52 |
| 1.430 | 2 | 7 2 0 | 65.18 |
| 1.418 | 1 | 2 7 1 | 65.82 |
| 1.416 | 2 | 1 5 2 | 65.93 |
| 1.390 | 2 | 5 6 0 | 67.32 |
| 1.376 | 1 | 7 3 0 | 68.11 |
| 1.369 | 1 | 5 1 2 | 68.47 |
| 1.367 | 2 | 6 4 1 | 68.62 |
| 1.363 | 1 | 7 1 1 | 68.83 |
| 1.327 | 2 | 4 4 2 | 70.97 |
| 1.317 | 2 | 0 6 2 | 71.59 |
| 1.306 | 9 | 1 6 2 | 72.26 |
| 1.301 | 1 | 5 6 1 | 72.61 |
| 1.294 | 2 | 8 0 0 | 73.08 |
| 1.285 | 1 | 8 1 0 | 73.64 |
| 1.281 | 1 | 4 7 1 | 73.94 |
| 1.254 | 1 | 6 1 2 | 75.81 |
| 1.241 | 2 | 1 9 0 | 76.73 |
| 1.234 | 1 | 7 4 1 | 77.26 |
| 1.231 | 1 | 6 2 2 | 77.47 |
| 1.230 | 1 | 3 6 2 | 77.52 |
| 1.214 | 1 | 8 1 1 | 78.76 |
| 1.201 | 2 | 6 6 1 | 79.81 |
| 1.200 | 5 | 2 0 3 | 79.89 |
| 1.196 | 4 | 6 3 2 | 80.21 |
| 1.193 | 1 | 8 2 1 | 80.40 |
| 1.177 | 4 | 1 9 1 | 81.79 |
| 1.176 | 1 | 5 5 2 | 81.84 |
| 1.176 | 1 | 4 7 0 | 81.85 |
| 1.175 | 1 | 8 4 0 | 81.89 |
| 1.175 | 3 | 3 9 0 | 81.90 |
| 1.174 | 2 | 4 6 2 | 82.04 |
| 1.172 | 2 | 7 5 1 | 82.18 |
| 1.172 | 3 | 0 3 3 | 82.21 |
| 1.164 | 1 | 1 3 3 | 82.85 |

| d (\AA) | I | hkl | 2θ ($^\circ$) $\lambda = 1.54056 \text{\AA}$ |
|----------------------|-----|--------|--|
| 1.161 | 2 | 8 3 1 | 83.11 |
| 1.151 | 1 | 6 4 2 | 84.00 |
| 1.149 | 1 | 7 1 2 | 84.20 |
| 1.131 | 1 | 7 2 2 | 85.82 |
| 1.120 | 3 | 3 9 1 | 86.90 |
| 1.111 | 2 | 5 6 2 | 87.78 |
| 1.110 | 1 | 5 8 1 | 87.92 |
| 1.109 | 1 | 3 3 3 | 87.95 |
| 1.108 | 2 | 7 6 1 | 88.11 |
| 1.104 | 1 | 7 3 2 | 88.51 |
| 1.093 | 1 | 9 1 1 | 89.62 |
| 1.078 | 1 | 9 2 1 | 91.23 |
| 1.070 | 1 | 5 9 0 | 92.09 |
| 1.067 | 6 | 4 3 3 | 92.39 |
| 1.060 | 2 | 6 0 2 | 93.19 |
| 1.056 | 1 | 8 1 2 | 93.73 |
| 1.044 | 1 | 7 7 1 | 95.10 |
| 1.041 | 1 | 5 2 3 | 95.43 |
| 1.031 | 2 | 1 9 2 | 96.73 |
| 1.028 | 4 | 5 9 1 | 97.07 |
| 1.025 | 3 | 1 6 3 | 97.40 |
| 1.024 | 1 | 9 5 0 | 97.57 |
| 1.020 | 1 | 5 3 3 | 98.13 |
| 1.011 | 1 | 2 6 3 | 99.32 |
| 1.003 | 2 | 6 0 3 | 100.31 |
| .993 | 1 | 10 1 1 | 101.76 |
| .992 | 1 | 6 7 2 | 101.83 |
| .992 | 1 | 8 4 2 | 101.87 |
| .992 | 4 | 3 9 2 | 101.88 |
| .987 | 3 | 3 6 3 | 102.55 |
| .972 | 2 | 8 7 1 | 104.78 |
| .962 | 1 | 9 2 2 | 106.35 |
| .959 | 1 | 8 5 2 | 106.86 |
| .955 | 1 | 5 10 1 | 107.53 |
| .955 | 1 | 7 9 0 | 107.59 |
| .945 | 1 | 6 4 3 | 109.20 |
| .939 | 2 | 10 4 1 | 110.15 |
| .934 | 1 | 1 12 0 | 111.18 |
| .926 | 1 | 5 9 2 | 112.53 |
| .925 | 2 | 0 0 4 | 112.76 |
| .923 | 1 | 8 6 2 | 113.16 |
| .923 | 1 | 9 4 2 | 113.21 |
| .911 | 2 | 10 5 1 | 115.39 |

CUMULATIVE INORGANIC INDEX

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|---|-----------------|------|
| Aluminum, Al | 1 | 11 | Ammonium iron sulfate hydrate, $\text{NH}_4\text{Fe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 10 |
| Aluminum antimony, AlSb | 4 | 72 | Ammonium lead chloride, $(\text{NH}_4)_2\text{PbCl}_6$ | 11m | 10 |
| Aluminum bismuth oxide, $\text{Al}_4\text{Bi}_2\text{O}_9$ | 11m | 5 | Ammonium magnesium aluminum fluoride, $\text{NH}_4\text{MgAlF}_6$ | 10m | 9 |
| Aluminum chloride, AlCl_3 | 9m | 61 | Ammonium manganese chloride hydrate, $(\text{NH}_4)_2\text{MnCl}_4 \cdot 2\text{H}_2\text{O}$ | 11m | 11 |
| Aluminum chloride hydrate (chloraluminite), $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ | 7 | 3 | Ammonium magnesium chromium oxide hydrate, $(\text{NH}_4)_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 10 |
| Aluminum fluoride hydroxide silicate, topaz, $\text{Al}_2(\text{F},\text{OH})_5\text{SiO}_4$ | 1m | 4 | Ammonium manganese(II) fluoride, NH_4MnF_3 | 5m | 8 |
| Aluminum nitrate hydrate, $\text{Al}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ | 11m | 6 | Ammonium manganese sulfate, $(\text{NH}_4)_2\text{Mn}(\text{SO}_4)_2$ | 7m | 8 |
| Aluminum oxide, (corundum), alpha Al_2O_3 | 9 | 3 | Ammonium manganese sulfate hydrate, $(\text{NH}_4)_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 12 |
| Aluminum oxide hydrate (böhmite), alpha $\text{Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ | 3 | 38 | Ammonium mercury chloride, NH_4HgCl_3 (revised) | 8m | 14 |
| Aluminum oxide hydrate, diaspore, beta $\text{Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ | 3 | 41 | Ammonium molybdenum oxide phosphate hydrate, $(\text{NH}_4)_2(\text{MoO}_3)_{12}\text{PO}_4 \cdot 4\text{H}_2\text{O}$ | 8 | 10 |
| Aluminum phosphate, $\text{Al}(\text{PO}_4)_3$ | 2m | 3 | Ammonium nickel(II) chloride, NH_4NiCl_3 | 6m | 6 |
| Aluminum phosphate (berlinite), AlPO_4 (trigonal) | 10 | 3 | Ammonium nickel chromium oxide hydrate, $(\text{NH}_4)_2\text{Ni}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 16 |
| Aluminum phosphate, AlPO_4 (orthorhombic) | 10 | 4 | Ammonium nitrate (ammonia-niter), NH_4NO_3 | 7 | 4 |
| Aluminum silicate (mullite) $3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2$ | 3m | 3 | Ammonium osmium bromide, $(\text{NH}_4)_2\text{OsBr}_6$ | 3 | 71 |
| Aluminum tungsten oxide, $\text{Al}_2(\text{WO}_4)_3$ | 11m | 7 | Ammonium osmium chloride, $(\text{NH}_4)_2\text{OsCl}_6$ | 1m | 6 |
| Ammonium aluminum fluoride, $(\text{NH}_4)_2\text{AlF}_6$ | 9m | 5 | Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_4$ | 6 | 6 |
| Ammonium aluminum selenate hydrate, $\text{NH}_4\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 9m | 6 | Ammonium palladium chloride, $(\text{NH}_4)_2\text{PdCl}_6$ | 8 | 7 |
| Ammonium aluminum sulfate, $\text{NH}_4\text{Al}(\text{SO}_4)_2$ | 10m | 5 | Ammonium platinum bromide, $(\text{NH}_4)_2\text{PtBr}_6$ | 9 | 6 |
| Ammonium aluminum sulfate hydrate (tschermigite), $\text{NH}_4\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 3 | Ammonium platinum chloride, $(\text{NH}_4)_2\text{PtCl}_6$ | 5 | 3 |
| Ammonium azide, NH_4N_3 | 9 | 4 | Ammonium rhenium oxide, NH_4ReO_4 | 9 | 7 |
| Ammonium beryllium fluoride, $(\text{NH}_4)_2\text{BeF}_4$ | 3m | 5 | Ammonium selenium bromide, $(\text{NH}_4)_2\text{SeBr}_6$ | 8 | 4 |
| Ammonium boron fluoride, NH_4BF_4 | 3m | 6 | Ammonium silicon fluoride (cryptohalite), $(\text{NH}_4)_2\text{SiF}_6$ | 5 | 5 |
| Ammonium bromide, NH_4Br | 2 | 49 | Ammonium sulfate (mascagnite), $(\text{NH}_4)_2\text{SO}_4$ (revised) | 9 | 8 |
| Ammonium cadmium chloride, NH_4CdCl_3 | 5m | 6 | Ammonium tellurium bromide, $(\text{NH}_4)_2\text{TeBr}_6$ | 8 | 5 |
| Ammonium cadmium sulfate, $(\text{NH}_4)_2\text{Cd}(\text{SO}_4)_2$ | 7m | 5 | Ammonium tellurium chloride, $(\text{NH}_4)_2\text{TeCl}_6$ | 8 | 8 |
| Ammonium cadmium sulfate hydrate, $(\text{NH}_4)_2\text{Cd}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 5 | Ammonium tin chloride, $(\text{NH}_4)_2\text{SnCl}_6$ | 5 | 4 |
| Ammonium calcium sulfate, $(\text{NH}_4)_2\text{Ca}_2(\text{SO}_4)_3$ | 8m | 7 | Ammonium vanadium oxide, NH_4VO_3 | 8 | 9 |
| Ammonium chlorate, NH_4ClO_4 (orthorhombic) | 7 | 6 | Ammonium zinc fluoride, NH_4ZnF_3 | 8m | 18 |
| Ammonium chloride (sal-ammoniac), NH_4Cl | 1 | 59 | Ammonium zirconium fluoride, $(\text{NH}_4)_2\text{ZrF}_7$ | 6 | 14 |
| Ammonium chromium sulfate hydrate, $\text{NH}_4\text{Cr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 7 | Antimony(III) fluoride, SbF_3 | 2m | 4 |
| Ammonium cobalt (II) chloride, NH_4CoCl_3 | 6m | 5 | Antimony(III) iodide, SbI_3 | 6 | 16 |
| Ammonium cobalt fluoride, NH_4CoF_3 | 8m | 9 | Antimony(III) oxide (senarmontite), Sb_2O_3 (cubic) | 3 | 31 |
| Ammonium copper bromide hydrate, $(\text{NH}_4)_2\text{CuBr}_4 \cdot 2\text{H}_2\text{O}$ | 10m | 6 | Antimony(III) oxide, valentinite, Sb_2O_3 (orthorhombic) | 10 | 6 |
| Ammonium copper chloride, NH_4CuCl_3 | 7m | 7 | Antimony(IV) oxide (cervantite), Sb_2O_4 | 10 | 8 |
| Ammonium copper chloride hydrate, $(\text{NH}_4)_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ | 9m | 8 | Antimony(V) oxide, Sb_2O_5 | 10 | 10 |
| Ammonium copper fluoride, NH_4CuF_3 | 11m | 8 | Antimony, Sb | 3 | 14 |
| Ammonium gallium sulfate hydrate, $\text{NH}_4\text{Ga}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 9 | Antimony selenide, Sb_2Se_3 | 3m | 7 |
| Ammonium germanium fluoride, $(\text{NH}_4)_2\text{GeF}_6$ | 6 | 8 | Antimony (III) sulfide (stibnite), Sb_2S_3 | 5 | 6 |
| Ammonium hydrogen carbonate (teschermache- rite), $(\text{NH}_4)\text{HCO}_3$ | 9 | 5 | Antimony telluride, Sb_2Te_3 | 3m | 8 |
| Ammonium hydrogen phosphate, $\text{NH}_4\text{H}_2\text{PO}_4$ | 4 | 64 | Arsenic, As | 3 | 6 |
| Ammonium iodate, NH_4IO_3 | 10m | 7 | Arsenic acid, $\text{H}_5\text{As}_3\text{O}_{10}$ | 7m | 84 |
| Ammonium iodide, NH_4I | 4 | 56 | Arsenic(III) iodide, AsI_3 | 6 | 17 |
| Ammonium iridium chloride, $(\text{NH}_4)_2\text{IrCl}_6$ | 8 | 6 | Arsenic oxide (arsenolite), As_2O_3 (cubic) | 1 | 51 |
| Ammonium iron fluoride, $(\text{NH}_4)_2\text{FeF}_6$ | 9m | 9 | Arsenic oxide, claudetite, As_2O_3 (mono-clinic) | 3m | 9 |
| Ammonium iron sulfate, $\text{NH}_4\text{Fe}(\text{SO}_4)_2$ | 10m | 8 | Barium, Ba | 4 | 7 |
| <hr/> | | | | | |
| * 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

| | Vol. or sec. | Page | Vol. or sec. | Page | |
|--|-----------------|------|--|------|----|
| Barium bromide hydrate, $\text{BaBr}_2 \cdot \text{H}_2\text{O}$ | 3m | 10 | Cadmium bromide, CdBr_2 | 9 | 17 |
| Barium calcium tungsten oxide, Ba_2CaWO_6 | 9m | 10 | Cadmium bromide chloride, CdBrCl | 11m | 15 |
| Barium carbonate (witherite), BaCO_3 , (orthorhombic) | 2 | 54 | Cadmium carbonate (otavite), CdCO_3 | 7 | 11 |
| Barium carbonate, BaCO_3 (cubic) at 1075 °C | 10 | 11 | Cadmium chlorate hydrate, $\text{Cd}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 3m | 19 |
| Barium chlorate hydrate, $\text{Ba}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$ | 2m | 7 | Cadmium chloride, CdCl_2 | 9 | 18 |
| Barium chloride hydrate, $\text{Ba}(\text{ClO}_3)_2 \cdot \text{H}_2\text{O}$ | 8m | 21 | Cadmium chromium oxide, CdCr_2O_4 | 5m | 16 |
| Barium chloride, BaCl_2 , (orthorhombic) | 9m | 11 | Cadmium cyanide, $\text{Cd}(\text{CN})_2$ | 2m | 8 |
| Barium chloride, BaCl_2 , (cubic) | 9m | 13 | Cadmium fluoride, CdF_2 | 10m | 15 |
| Barium chloride fluoride, BaClF | 10m | 11 | Cadmium iron oxide, CdFe_2O_4 | 9m | 16 |
| Barium fluoride, BaF_2 | 1 | 70 | Cadmium manganese oxide, CdMn_2O_4 | 10m | 16 |
| Barium hydroxide phosphate, $\text{Ba}_3(\text{OH})(\text{PO}_4)_3$ | 11m | 12 | Cadmium molybdenum oxide, CdMoO_4 | 6 | 21 |
| Barium iodide, BaI_2 | 10m | 66 | Cadmium nitrate hydrate, $\text{Cd}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$ | 7m | 93 |
| Barium lead chloride, BaPbCl_4 | 11m | 13 | Cadmium oxide, CdO | 2 | 27 |
| Barium molybdenum oxide, BaMoO_4 | 7 | 7 | Cadmium oxide, CdO (ref. standard) | 8m | 2 |
| Barium nitrate (nitrobarite), $\text{Ba}(\text{NO}_3)_2$ (revised) | 11m | 14 | Cadmium selenide, CdSe (hexagonal) | 7 | 12 |
| Barium oxide, BaO | 9m | 63 | Cadmium sulfate, CdSO_4 | 3m | 20 |
| Barium oxide, BaO_2 | 6 | 18 | Cadmium sulfate hydrate, $3\text{CdSO}_4 \cdot 8\text{H}_2\text{O}$ | 6m | 8 |
| Barium selenide, BaSe | 5m | 61 | Cadmium sulfate hydrate, $\text{CdSO}_4 \cdot \text{H}_2\text{O}$ | 6m | 10 |
| Barium silicon fluoride, BaSiF_6 | 4m | 7 | Cadmium sulfide (greenockite), CdS | 4 | 15 |
| Barium sulfate (barite), BaSO_4 (revised) | 10m | 12 | Cadmium telluride, CdTe | 3m | 21 |
| Barium sulfide, BaS | 7 | 8 | Cadmium tungsten oxide, CdWO_4 | 2m | 8 |
| Barium tin oxide, BaSnO_3 | 3m | 11 | Calcium, Ca | 9m | 68 |
| Barium titanium oxide, BaTiO_3 | 3 | 45 | Calcium aluminum germanium oxide, $\text{Ca}_3\text{Al}_2(\text{GeO}_4)_3$ | 10 | 15 |
| Barium titanium silicate (fresnoite), $\text{Ba}_2\text{TiSi}_2\text{O}_8$ | 9m | 14 | Calcium aluminum hydroxide, $\text{Ca}_3\text{Al}_2(\text{OH})_{12}$ | 11m | 16 |
| Barium tungsten oxide, BaWO_4 | 7 | 9 | Calcium aluminum oxide, $\text{Ca}_3\text{Al}_2\text{O}_6$ | 5 | 10 |
| Barium zirconium oxide, BaZrO_3 | 5 | 8 | Calcium aluminum oxide, $12\text{CaO} \cdot 7\text{Al}_2\text{O}_3$ | 9 | 20 |
| Beryllium, alpha, Be | 9m | 64 | Calcium aluminum sulfate hydrate (ettringite), $6\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 3\text{SO}_4 \cdot 31\text{H}_2\text{O}$ | 8 | 3 |
| Beryllium aluminum oxide (chrysoberyl), BeAl_2O_4 | 9 | 10 | Calcium Bromide, CaBr_2 | 11m | 70 |
| Beryllium aluminum silicate, beryl, $\text{Be}_3\text{Al}_2(\text{SiO}_4)_6$ | 9 | 13 | Calcium bromide hydrate, $\text{CaBr}_2 \cdot 6\text{H}_2\text{O}$ | 8 | 15 |
| Beryllium calcium oxide, $\text{Be}_{1-x}\text{Ca}_x\text{O}$ | 7m | 89 | Calcium carbonate (aragonite), CaCO_3 (orthorhombic) | 3 | 53 |
| Beryllium chromium oxide, BeCr_2O_4 | 10 | 12 | Calcium carbonate (calcite) CaCO_3 (hexagonal) | 2 | 51 |
| Beryllium cobalt, BeCo | 5m | 62 | Calcium chloride fluoride, CaClF | 10m | 17 |
| Beryllium germanium oxide, Be_2GeO_4 | 10 | 13 | Calcium chloride (hydrophilite), CaCl_2 | 11m | 18 |
| Beryllium lanthanum oxide, $\text{Be}_2\text{La}_2\text{O}_5$ | 9m | 65 | Calcium chloride hydrate, $\text{CaCl}_2 \cdot 4\text{H}_2\text{O}$ | 11m | 73 |
| Beryllium niobium, Be_2Nb | 7m | 92 | Calcium chromium germanium oxide, $\text{Ca}_3\text{Cr}_2(\text{GeO}_4)_3$ | 10 | 16 |
| Beryllium oxide (bromellite), BeO | 1 | 36 | Calcium chromium oxide, CaCrO_4 | 7 | 13 |
| Beryllium palladium, BePd | 5m | 62 | Calcium chromium silicate (uvarovite), $\text{Ca}_3\text{Cr}_2(\text{SiO}_4)_3$ | 10 | 17 |
| Beryllium silicate, phenacite, BeSi_2O_4 | 8 | 11 | Calcium fluoride (fluorite), CaF_2 | 1 | 69 |
| Bismuth, Bi | 3 | 20 | Calcium fluoride phosphate (fluorapatite), $\text{Ca}_5\text{F}(\text{PO}_4)_3$ | 3m | 22 |
| Bismuth fluoride, BiF_3 | 1m | 7 | Calcium gallium germanium oxide, $\text{Ca}_3\text{Ga}_2(\text{GeO}_4)_3$ | 10 | 18 |
| Bismuth(III) iodide, BiI_3 | 6 | 20 | Calcium hydroxide (portlandite), $\text{Ca}(\text{OH})_2$ | 1 | 58 |
| Bismuth oxide (bismite), alpha Bi_2O_3 | 3m | 16 | Calcium iron germanium oxide, $\text{Ca}_3\text{Fe}_2(\text{GeO}_4)_3$ | 10 | 19 |
| Bismuth oxide bromide, BiOBr | 8 | 14 | Calcium iron silicate (andradite), $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_12$ | 9 | 22 |
| Bismuth oxide chloride (bismoclite), BiOCl | 4 | 54 | Calcium iron silicate hydroxide, julgoldite, $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_10(\text{OH},\text{O})_2(\text{OH})_2$ | 10m | 72 |
| Bismuth oxide iodide, BiOI | 9 | 16 | Calcium magnesium silicate (diopside), $\text{CaMg}(\text{SiO}_3)_2$ | 5m | 17 |
| Bismuth phosphate, BiPO_4 (monoclinic) | 3m | 11 | Calcium molybdenum oxide (powellite), CaMoO_4 | 6 | 22 |
| Bismuth phosphate, BiPO_4 (trigonal) | 3m | 13 | Calcium nitrate, $\text{Ca}(\text{NO}_3)_2$ | 7 | 14 |
| Bismuth sulfide (bismuthinite), Bi_2S_3 (revised) | 5m | 13 | Calcium oxide, CaO | 1 | 43 |
| Bismuth telluride, BiTe | 4m | 50 | Calcium phosphate, beta $\text{Ca}_2\text{P}_2\text{O}_7$ | 7m | 95 |
| Bismuth telluride (tellurobismuthite), Bi_2Te_3 | 3m | 16 | Calcium platinum oxide, Ca_4PtO_6 | 10m | 18 |
| Bismuth vanadium oxide, low form, BiVO_4 (tetragonal) | 3m | 14 | Calcium selenide, CaSe | 5m | 64 |
| Bismuth vanadium oxide, high form, BiVO_4 (monoclinic) | 3m | 14 | Calcium sulfate (anhydrite), CaSO_4 | 4 | 65 |
| Boric acid, HBO_2 (cubic) | 4m | 27 | Calcium sulfate (oldhamite), CaS | 7 | 15 |
| Boron oxide, B_2O_3 , phase 1 | 10m | 70 | Calcium telluride, CaTe | 4m | 50 |
| Cadmium, Cd | 3 | 10 | | | |
| Cadmium ammine chloride, $\text{Cd}(\text{NH}_3)\text{Cl}_2$ | 10m | 14 | | | |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|--|-----------------|------|
| Calcium titanium oxide (perovskite), CaTiO_3 | 9m | 17 | Cesium lithium fluoride, CsLiF_x | 7m | 105 |
| Calcium tungsten oxide, Ca_2WO_6 | 9m | 19 | Cesium magnesium chromium oxide, $\text{Cs}_2\text{Mg}_2(\text{CrO}_4)_3$ | 8m | 27 |
| Calcium tungsten oxide, scheelite, CaWO_4 | 6 | 23 | Cesium magnesium chromium oxide hydrate, $\text{Cs}_2\text{Mg}(\text{CrO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 8m | 29 |
| Carbon, diamond, C | 2 | 5 | Cesium manganese fluoride, CsMnF_3 | 10m | 21 |
| Cerium antimony, CeSb | 4m | 40 | Cesium magnesium sulfate hydrate, $\text{Cs}_2\text{Mg}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 18 |
| Cerium arsenate, CeAsO_4 | 4m | 8 | Cesium manganese sulfate hydrate, $\text{Cs}_2\text{Mn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 20 |
| Cerium arsenide, CeAs | 4m | 51 | Cesium mercury chloride, CsHgCl_1 | 7m | 22 |
| Cerium bismuth, CeBi | 4m | 46 | Cesium nickel(II) chloride, CsNiCl_3 | 6m | 12 |
| Cerium cadmium, CeCd | 5m | 63 | Cesium nickel sulfate hydrate, $\text{Cs}_2\text{Ni}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 23 |
| Cerium(III) chloride, CeCl_3 | 1m | 8 | Cesium nitrate, CsNO_3 | 9 | 25 |
| Cerium copper, CeCu_x | 7m | 99 | Cesium osmium(IV) bromide, Cs_2OsBr_6 | 2m | 10 |
| Cerium(III) fluoride, CeF_3 | 8 | 17 | Cesium osmium chloride, Cs_2OsCl_6 | 2m | 11 |
| Cerium niobium titanium oxide (eschynite), CeNbTiO_6 | 3m | 24 | Cesium platinum bromide, Cs_2PtBr_6 | 8 | 19 |
| Cerium nitride, CeN | 4m | 51 | Cesium platinum chloride, Cs_2PtCl_6 | 5 | 14 |
| Cerium(IV) oxide (cerianite), CeO_2 | 1 | 56 | Cesium platinum fluoride, Cs_2PtF_6 | 6 | 27 |
| Cerium phosphide, CeP | 4m | 52 | Cesium selenium bromide, Cs_2SeBr_6 | 8 | 20 |
| Cerium(III) vanadium oxide, CeVO_4 | 1m | 9 | Cesium silicon fluoride, Cs_2SiF_6 | 5 | 19 |
| Cerium zinc, CeZn | 5m | 65 | Cesium strontium chloride, CsSrCl_3 | 6m | 13 |
| Cesium aluminum sulfate hydrate, $\text{CsAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 25 | Cesium sulfate Cs_2SO_4 | 7 | 17 |
| Cesium antimony fluoride, CsSbF_6 | 4m | 9 | Cesium tellurium bromide, Cs_2TeBr_6 | 9 | 24 |
| Cesium beryllium fluoride, CsBeF_3 | 9m | 69 | Cesium tin chloride, Cs_2SnCl_6 | 5 | 16 |
| Cesium boron fluoride, CsBF_4 | 8 | 22 | Cesium vanadium sulfate hydrate, $\text{CsV}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 1m | 11 |
| Cesium bromate, CsBrO_3 | 8 | 18 | Cesium zinc sulfate hydrate, $\text{Cs}_2\text{Zn}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 25 |
| Cesium bromide, CsBr | 3 | 49 | Chromium, Cr | 5 | 20 |
| Cesium cadmium bromide, CsCdBr_3 (hexagonal) | 10m | 20 | Chromium chloride, CrCl_2 | 11m | 77 |
| Cesium cadmium chloride, CsCdCl_3 , (hexagonal) | 5m | 19 | Chromium fluoride, Cr_2F_8 | 7m | 108 |
| Cesium calcium chloride, CsCaCl_3 | 5m | 21 | Chromium fluoride, CrF_2 | 10m | 81 |
| Cesium calcium fluoride, CsCaF_3 | 8m | 25 | Chromium(III) fluoride hydrate, $\text{CrF}_3 \cdot 3\text{H}_2\text{O}$ | 5m | 25 |
| Cesium calcium sulfate, $\text{Cs}_2\text{Ca}(\text{SO}_4)_2$ | 7m | 12 | Chromium iridium 3:1, Cr_3Ir | 6m | 14 |
| Cesium cerium chloride, Cs_2CeCl_6 | 7m | 101 | Chromium(III) oxide, Cr_2O_3 | 5 | 22 |
| Cesium chloride, CsClO_4 | 8 | 20 | Chromium phosphate, alpha CrPO_4 | 2m | 12 |
| Cesium chloride, CsClO_4 (orthorhombic) | 1m | 10 | Chromium phosphate, beta CrPO_4 | 9 | 26 |
| Cesium chloride, CsCl | 2 | 44 | Chromium rhodium 3:1, Cr_3Rh | 6m | 15 |
| Cesium chromium oxide, Cs_2CrO_4 | 3m | 25 | Chromium silicide, Cr_3Si | 6 | 29 |
| Cesium chromium sulfate hydrate, $\text{CsCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 8 | 21 | Cobalt, Co (cubic) | 4m | 10 |
| Cesium cobalt(II) chloride, CsCoCl_3 | 6m | 11 | Cobalt aluminum oxide, CoAl_2O_4 | 9 | 27 |
| Cesium cobalt chloride, Cs_2CoCl_4 | 11m | 19 | Cobalt ammine iodide, $\text{Co}(\text{NH}_3)_6\text{I}_3$ | 10m | 83 |
| Cesium copper(II) chloride, CsCuCl_2 | 5m | 22 | Cobalt antimony oxide, CoSb_2O_6 | 5m | 26 |
| Cesium copper chloride, Cs_2CuCl_4 | 11m | 20 | Cobalt arsenide, CoAs_2 (revised) | 4m | 10 |
| Cesium copper sulfate hydrate, $\text{Cs}_2\text{Cu}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 14 | Cobalt arsenide (skutterudite), CoAs_3 | 10 | 21 |
| Cesium fluoride, CsF | 3m | 26 | Cobalt(II) carbonate (spherocobaltite), CoCO_3 | 10 | 24 |
| Cesium gallium sulfate hydrate, $\text{CsGa}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 8 | 23 | Cobalt chlorate hydrate, $\text{Co}(\text{ClO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 3m | 28 |
| Cesium germanium fluoride, Cs_2GeF_6 | 5 | 17 | Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 22 |
| Cesium iodide, CsI | 4 | 47 | Cobalt chloride hydrate, $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ | 11m | 23 |
| Cesium iodine bromide, CsI_3Br | 7m | 103 | Cobalt chromium oxide, CoCr_2O_4 | 9m | 21 |
| Cesium iodine chloride, CsICl_2 | 3 | 50 | Cobalt fluoride, CoF_3 | 10m | 85 |
| Cesium iron sulfate hydrate, $\text{Cs}_2\text{Fe}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ | 7m | 16 | Cobalt fluoride hydrate, $\text{CoF}_2 \cdot 4\text{H}_2\text{O}$ | 11m | 24 |
| Cesium iron sulfate hydrate, $\text{CsFe}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 28 | Cobalt gallium oxide, CoGa_2O_4 | 10 | 27 |
| Cesium lead(II) chloride, CsPbCl_3 , (tetragonal) | 5m | 24 | Cobalt germanium oxide, Co_2GeO_4 | 10 | 27 |
| Cesium lead fluoride, CsPbF_6 | 8m | 26 | Cobalt iodide, CoI_2 | 4m | 52 |
| Cesium lithium cobalt cyanide, $\text{CsLiCo}(\text{CN})_6$ | 10m | 79 | Cobalt iron arsenide (safflorite), CoFeAs_3 | 10 | 28 |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|--|-----------------|------|
| Cobalt sulfate, beta, CoSO_4 | 2m | 14 | Gadolinium gallium oxide, $\text{Gd}_3\text{Ga}_2(\text{GaO}_4)_3$ | 2m | 18 |
| Cobalt titanium oxide, CoTiO_3 | 4m | 13 | Gadolinium indium, GdIn | 5m | 67 |
| Cobalt tungsten oxide, CoWO_4 | 4m | 13 | Gadolinium nitride, GdN | 4m | 57 |
| Copper, Cu | 1 | 15 | Gadolinium oxide, Gd_2O_3 | 1m | 16 |
| Copper aluminum, Cu_2Al_4 | 11m | 79 | Gadolinium oxychloride, GdOCl | 1m | 17 |
| Copper ammine selenate, $\text{Cu}(\text{NH}_3)_4\text{SeO}_4$ | 10m | 87 | Gadolinium silver, GdAg | 6m | 87 |
| Copper ammine sulfate hydrate, $\text{Cu}(\text{NH}_3)_4\text{SO}_4 \cdot 2\text{H}_2\text{O}$ | 10m | 90 | Gadolinium titanium oxide, Gd_2TiO_5 | 8m | 32 |
| Copper antimony oxide, CuSb_2O_6 | 5m | 27 | Gadolinium vanadium oxide, GdVO_4 | 5m | 30 |
| Copper(I) bromide, CuBr | 4 | 36 | Gallium, Ga | 2 | 9 |
| Copper cadmium, Cu_3Cd_5 | 11m | 81 | Gallium antimony, GaSb | 6 | 30 |
| Copper (I) chloride (nantokite), CuCl | 4 | 35 | Gallium arsenide, GaAs | 3m | 33 |
| Copper fluoride hydrate, $\text{CuF}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 25 | Gallium oxide, alpha, Ga_2O_3 | 4 | 25 |
| Copper hydrogen phosphite hydrate, $\text{CuHPO}_3 \cdot 2\text{H}_2\text{O}$ | 11m | 83 | Gallium phosphate hydrate, $\text{GaPO}_4 \cdot 2\text{H}_2\text{O}$ | 8m | 34 |
| Copper hydroxide carbonate, azurite, $\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2$ | 10 | 30 | Gallium phosphate (α -quartz type), GaPO_4 | 8 | 27 |
| Copper hydroxide carbonate (malachite), $\text{Cu}_2(\text{OH})_2\text{CO}_3$ | 10 | 31 | Germanium, Ge | 1 | 18 |
| Copper(I) iodide (marchite), CuI | 4 | 38 | Germanium iodide, GeI_2 | 4m | 58 |
| Copper (I) oxide (cuprite), Cu_2O | 2 | 23 | Germanium(IV) iodide, GeI_4 | 5 | 25 |
| Copper(II) oxide (tenorite), CuO | 1 | 49 | Germanium oxide, GeO_2 (hexagonal) (low form) | 1 | 51 |
| Copper phosphate, alpha $\text{Cu}_2\text{P}_2\text{O}_7$ | 7m | 113 | Germanium oxide, GeO_2 (tetragonal) (high form) | 8 | 28 |
| Copper sulfate (chalcocyanite), CuSO_4 | 3m | 29 | Gold, Au | 1 | 33 |
| Copper(II) sulfide (covellite), CuS | 4 | 13 | Gold antimony 1:2 (aurostibite), AuSb_2 | 7 | 18 |
| Copper uranium oxide, CuUO_4 | 10m | 93 | Gold(I) cyanide, AuCN | 10 | 33 |
| Dysprosium antimony, DySb | 4m | 41 | Gold potassium cyanide, AuK(CN)_2 | 8m | 36 |
| Dysprosium arsenate, DyAsO_4 | 3m | 30 | Gold tin, 1:1 AuSn | 7 | 19 |
| Dysprosium arsenide, DyAs | 4m | 53 | Gold titanium 1:3, AuTi_3 | 6m | 17 |
| Dysprosium bismuth, DyBi | 4m | 47 | Hafnium, Hf | 3 | 18 |
| Dysprosium gallium oxide, $\text{Dy}_3\text{Ga}_5(\text{GaO}_4)_3$ | 2m | 15 | Holmium arsenate, HoAsO_4 | 3m | 34 |
| Dysprosium gold, DyAu | 5m | 66 | Holmium bismuth, HoBi | 4m | 48 |
| Dysprosium nitride, DyN | 4m | 53 | Holmium fluoride, HoF_3 | 10m | 23 |
| Dysprosium oxide, Dy_2O_3 | 9 | 30 | Holmium gold, HoAu | 5m | 68 |
| Dysprosium silver, DyAg | 5m | 66 | Holmium nitride, HoN | 4m | 58 |
| Dysprosium telluride, DyTe | 4m | 54 | Holmium oxide, Ho_2O_3 | 9 | 32 |
| Dysprosium vanadium oxide, DyVO_4 | 4m | 15 | Holmium selenide, HoSe | 4m | 59 |
| Erbium antimony, ErSb | 4m | 41 | Holmium silver, HoAg | 5m | 68 |
| Erbium arsenate, ErAsO_4 | 3m | 31 | Holmium vanadium oxide, HoVO_4 | 4m | 18 |
| Erbium arsenide, ErAs | 4m | 54 | Hydrogen borate, beta HBO_2 | 9m | 71 |
| Erbium bismuth, ErBi | 4m | 47 | Hydrogen iodate, HIO_3 | 5 | 28 |
| Erbium gallium oxide, $\text{Er}_3\text{Ga}_5(\text{GaO}_4)_3$ | 1m | 12 | Hydrogen iodate, HI_3O_8 | 8m | 104 |
| Erbium manganese oxide, ErMnO_3 | 2m | 16 | Indium, In | 3 | 12 |
| Erbium nitride, ErN | 4m | 55 | Indium antimony, InSb | 4 | 73 |
| Erbium oxide, Er_2O_3 | 8 | 25 | Indium arsenide, InAs | 3m | 35 |
| Erbium phosphate, ErPO_4 | 9 | 31 | Indium oxide, In_2O_3 | 5 | 26 |
| Erbium silver, ErAg | 5m | 67 | Indium phosphate, InPO_4 | 8 | 29 |
| Erbium telluride, ErTe | 4m | 55 | Indium sulfide, In_2S_3 | 11m | 30 |
| Erbium vanadium oxide, ErVO_4 | 5m | 29 | Iodine, I_2 | 3 | 16 |
| Europium arsenate, EuAsO_4 | 3m | 32 | Iridium, Ir | 4 | 9 |
| Europium(III) chloride, EuCl_3 | 1m | 13 | Iridium oxide, IrO_2 | 4m | 19 |
| Europium gallium oxide, $\text{Eu}_3\text{Ga}_5(\text{GaO}_4)_3$ | 2m | 17 | Iridium titanium 1:3, IrTi_3 | 6m | 20 |
| Europium nitride, EuN | 4m | 56 | Iron, alpha Fe | 4 | 3 |
| Europium oxide, EuO | 4m | 56 | Iron arsenide, FeAs | 1m | 19 |
| Europium oxychloride, EuOCl | 1m | 13 | Iron arsenide (loellingite), FeAs_2 | 10 | 34 |
| Europium phosphate, EuPO_4 | 11m | 26 | Iron bromide, FeBr_3 | 4m | 59 |
| Europium(III) vanadium oxide, EuVO_4 | 4m | 16 | Iron chloride hydrate, $\text{FeCl}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 32 |
| Gadolinium antimony, GdSb | 4m | 42 | Iron fluoride hydrate, $\text{FeF}_2 \cdot 4\text{H}_2\text{O}$ | 11m | 90 |
| Gadolinium arsenate, GdAsO_4 | 4m | 17 | Iron hydroxide sulfate hydrate, butlerite, $\text{Fe(OH)}\text{SO}_4 \cdot 2\text{H}_2\text{O}$ | 10m | 95 |
| Gadolinium arsenide, GdAs | 4m | 57 | Iron iodide, FeI_2 | 4m | 60 |
| Gadolinium chloride hydrate, $\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$ | 7m | 118 | Iron(II,III) oxide (magnetite), Fe_3O_4 | 5m | 31 |
| Gadolinium fluoride, GdF_3 | 1m | 14 | Iron sulfate hydrate (melanterite), $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ | 8m | 38 |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|---|-----------------|------|
| Lanthanum borate, LaBO ₃ | 1m | 20 | Lithium phosphate, low form (lithiophosphate), Li ₂ PO ₄ (orthorhombic) revised | 4m | 21 |
| Lanthanum cadmium, LaCd | 5m | 63 | Lithium phosphate, high form, Li ₂ PO ₄ | 3m | 39 |
| Lanthanum chloride, LaCl ₃ | 1m | 20 | Lithium rubidium fluoride, LiRbF ₄ | 7m | 128 |
| Lanthanum fluoride, LaF ₃ | 7 | 21 | Lithium selenide, Li ₂ Se | 10m | 100 |
| Lanthanum niobium titanium oxide, LaNbTiO ₆ | 3m | 37 | Lithium sodium aluminum fluoride, cryolithionite, Li ₃ Na ₂ Al ₂ F ₁₂ | 9m | 23 |
| Lanthanum nitrate hydrate, La(NO ₃) ₃ ·6H ₂ O | 8m | 40 | Lithium sodium sulfate, LiNaSO ₄ | 6m | 24 |
| Lanthanum nitride, LaN | 4m | 61 | Lithium sulfate, Li ₂ SO ₄ | 6m | 26 |
| Lanthanum oxide, La ₂ O ₃ | 3 | 33 | Lithium sulfate hydrate, Li ₂ SO ₄ ·H ₂ O | 4m | 22 |
| Lanthanum oxychloride, LaOCl | 7 | 22 | Lithium sulfide, Li ₂ S | 10m | 101 |
| Lanthanum phosphide, LaP | 5m | 69 | Lithium telluride, Li ₂ Te | 10m | 102 |
| Lanthanum selenide, LaSe | 4m | 61 | Lithium tungsten oxide, Li ₂ WO ₄ (trigonal) | 1m | 25 |
| Lanthanum zinc, LaZn | 5m | 70 | Lithium tungsten oxide hydrate, Li ₂ WO ₄ ·½H ₂ O | 2m | 20 |
| Lead, Pb | 1 | 34 | Lithium uranium fluoride, LiUF ₄ | 7m | 131 |
| Lead borate, PbB ₄ O ₇ | 4m | 19 | Lutetium arsenate, LuAsO ₄ | 5m | 36 |
| Lead bromide, PbBr ₂ | 2 | 47 | Lutetium gallium oxide, Lu ₃ Ga ₂ (GaO ₄) ₃ | 2m | 22 |
| Lead bromide chloride, PbBrCl | 11m | 33 | Lutetium manganese oxide, LuMnO ₃ | 2m | 23 |
| Lead bromide fluoride, PbBrF ₃ | 10m | 25 | Lutetium nitride, LuN | 4m | 62 |
| Lead carbonate (cerussite), PbCO ₃ | 2 | 56 | Lutetium oxide, Lu ₂ O ₃ | 1m | 27 |
| Lead chloride (cotunnite), PbCl ₂ | 2 | 45 | Lutetium vanadium oxide, LuVO ₄ | 5m | 37 |
| Lead chloride fluoride (matlockite), PbClF ₃ | 1 | 76 | Magnesium, Mg | 1 | 10 |
| Lead fluoride, alpha PbF ₂ (orthorhombic) | 5 | 31 | Magnesium aluminum oxide (spinel), MgAl ₂ O ₄ (revised) | 9m | 25 |
| Lead fluoride, beta PbF ₂ (cubic) | 5 | 33 | Magnesium aluminum silicate (pyrope), Mg ₃ Al ₂ (SiO ₄) ₃ | 4m | 24 |
| Lead fluoride iodide, PbFI | 10m | 26 | Magnesium aluminum silicate (low cordierite), Mg ₂ Al ₄ Si ₅ O ₁₈ (orthorhombic) | 1m | 28 |
| Lead hydroxide phosphate, Pb ₅ (PO ₄) ₃ OH | 8 | 33 | Magnesium aluminum silicate (high cordierite), Mg ₂ Al ₄ Si ₅ O ₁₈ (hexagonal) | 1m | 29 |
| Lead(II) iodide, PbI ₂ | 5 | 34 | Magnesium ammonium phosphate hydrate, (struvite), MgNH ₄ PO ₄ ·6H ₂ O | 3m | 41 |
| Lead molybdenum oxide (wulfenite), PbMoO ₄ | 7 | 23 | Magnesium borate, Mg ₂ B ₂ O ₅ (triclinic) | 4m | 25 |
| Lead nitrate, Pb(NO ₃) ₂ | 5 | 36 | Magnesium bromide, MgBr ₂ | 4m | 62 |
| Lead oxide (litharge), PbO (red, tetragonal) | 2 | 30 | Magnesium bromide hydrate, MgBr ₂ ·6H ₂ O | 11m | 35 |
| Lead oxide (massicot), PbO (yellow, orthorhombic) | 2 | 32 | Magnesium carbonate (magnesite), MgCO ₃ | 7 | 28 |
| Lead(II, III) oxide (minium), Pb ₃ O ₄ | 8 | 32 | Magnesium cerium MgCe | 5m | 65 |
| Lead oxide sulfate, Pb ₃ O ₄ SO ₄ | 10m | 27 | Magnesium cerium nitrate hydrate, Mg ₂ Ce ₂ (NO ₃) ₁₂ ·24H ₂ O | 10 | 20 |
| Lead oxybromide, Pb ₃ O ₂ Br ₂ | 5m | 32 | Magnesium chlorate hydrate, Mg(ClO ₄) ₂ ·6H ₂ O | 7m | 30 |
| Lead selenide (clausthalite), PbSe | 5 | 38 | Magnesium chloride (chloromagnesite), MgCl ₂ | 11m | 94 |
| Lead sulfate (anglesite), PbSO ₄ | 3 | 67 | Magnesium chloride hydrate, MgCl ₂ ·12H ₂ O | 7m | 135 |
| Lead sulfide (galena), PbS | 2 | 18 | Magnesium chloride hydrate (bischofite), MgCl ₂ ·6H ₂ O | 11m | 37 |
| Lead tin oxide, Pb ₂ SnO ₄ | 10m | 29 | Magnesium chromium oxide (picrochromite), MgCr ₂ O ₄ | 9 | 34 |
| Lead titanium oxide, PbTiO ₃ | 5 | 39 | Magnesium fluoride (sellalite), MgF ₂ | 4 | 33 |
| Lead tungsten oxide (stolzite), PbWO ₄ (tetragonal) (revised) | 5m | 34 | Magnesium fluoride silicate (humite), Mg ₂ F ₂ (SiO ₄) ₃ | 1m | 30 |
| Lead uranium oxide, Pb ₃ UO ₈ | 8m | 109 | Magnesium fluoride silicate (norbergite), Mg ₃ F ₂ SiO ₄ | 10 | 39 |
| Letetium manganese oxide, LuMnO ₃ | 2m | 23 | Magnesium gallium oxide, MgGa ₂ O ₄ | 10 | 36 |
| Lithium aluminum, Li ₂ Al ₄ | 10m | 98 | Magnesium germanium oxide, Mg ₂ GeO ₄ (cubic) | 10 | 37 |
| Lithium aluminum fluoride, alpha Li ₂ AlF ₆ | 8m | 111 | Magnesium germanium oxide, Mg ₂ GeO ₄ (orthorhombic) | 10 | 38 |
| Lithium arsenate, Li ₂ AsO ₄ | 2m | 19 | Magnesium gold, MgAu | 6m | 83 |
| Lithium azide, Li ₂ N | 8m | 113 | Magnesium hydrogen phosphate hydrate, newberyite, MgHPO ₄ ·3H ₂ O | 7m | 139 |
| Lithium barium fluoride, LiBaF ₃ | 5m | 35 | Magnesium hydroxide (brucite), Mg(OH) ₂ | 6 | 30 |
| Lithium beryllium fluoride, Li ₂ BeF ₄ | 7m | 126 | Magnesium iron hydroxide carbonate hydrate, pyroaurite, Mg ₆ Fe ₂ (OH) ₁₆ CO ₄ ·4H ₂ O, phase II | 10m | 104 |
| Lithium borate, Li ₂ B ₄ O ₇ | 8m | 114 | Magnesium iron hydroxide carbonate hydrate, sjögrenite, Mg ₆ Fe ₂ (OH) ₁₆ CO ₄ ·4H ₂ O, phase I | 10m | 103 |
| Lithium bromide, LiBr | 4 | 30 | Magnesium lanthanum, MgLa | 5m | 69 |
| Lithium carbonate, Li ₂ CO ₃ | 8m | 42 | Magnesium lanthanum nitrate hydrate, Mg ₃ La ₂ (NO ₃) ₁₂ ·24H ₂ O | 1m | 22 |
| Lithium chlorate hydrate, LiClO ₄ ·3H ₂ O | 8 | 34 | | | |
| Lithium chloride, LiCl | 1 | 62 | | | |
| Lithium fluoride, LiF | 1 | 61 | | | |
| Lithium gallium oxide, LiGaO ₂ | 10m | 31 | | | |
| Lithium hydroxide hydrate, LiOH·H ₂ O | 11m | 92 | | | |
| Lithium iodate, LiIO ₃ | 7 | 26 | | | |
| Lithium iodate, LiIO ₃ (tetragonal) | 10m | 33 | | | |
| Lithium molybdenum oxide, Li ₂ MoO ₄ (trigonal) | 1m | 23 | | | |
| Lithium niobium oxide, LiNbO ₃ | 6m | 22 | | | |
| Lithium nitrate, LiNO ₃ | 7 | 27 | | | |
| Lithium oxide, Li ₂ O | 1m | 25 | | | |
| Lithium phosphate hydrate, Li ₂ P ₂ O ₇ ·3H ₂ O | 2m | 20 | | | |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|---|-----------------|------|
| Magnesium manganese oxide, $MgMn_2O_4$ | 10m | 35 | Molybdenum oxide (molybdate), MoO_3 | 3 | 30 |
| Magnesium mercury, $MgHg$ | 6m | 84 | Molybdenum sulfide (molybdenite), MoS_2 | 5 | 47 |
| Magnesium molybdenum oxide, $MgMoO_4$ | 7m | 28 | Neodymium antimony, $NdSb$ | 4m | 43 |
| Magnesium nickel oxide, $MgNiO_2$ | 10m | 36 | Neodymium arsenate, $NdAsO_4$ | 4m | 28 |
| Magnesium oxide (periclase), MgO | 1 | 37 | Neodymium arsenide, $NdAs$ | 4m | 64 |
| Magnesium phosphate, alpha $Mg_2P_2O_7$ | 9m | 73 | Neodymium bismuth, $NdBi$ | 4m | 49 |
| Magnesium selenide, $MgSe$ | 5m | 70 | Neodymium borate, $NdBO_3$ | 1m | 32 |
| Magnesium selenite hydrate, $MgSeO_3 \cdot 6H_2O$ | 8m | 116 | Neodymium chloride, $NdCl$ | 1m | 33 |
| Magnesium silicate, enstatite, $MgSiO_3$ | 6 | 32 | Neodymium fluoride, NdF | 8 | 36 |
| Magnesium silicate (forsterite), Mg_2SiO_4 | 1 | 83 | Neodymium gallium oxide, $Nd_3Ga_2(GaO_4)_3$ | 1m | 34 |
| Magnesium sulfate hydrate (epsomite), $MgSO_4 \cdot 7H_2O$ | 7 | 30 | Neodymium oxide, Nd_2O_3 | 4 | 26 |
| Magnesium sulfide, MgS | 7 | 31 | Neodymium oxychloride, $NdOCl$ | 8 | 37 |
| Magnesium sulfite hydrate, $MgSO_4 \cdot 6H_2O$ | 9m | 26 | Neodymium phosphate, $NdPO_4$ | 11m | 40 |
| Magnesium titanium oxide (geikielite), $MgTiO_3$ | 5 | 43 | Neodymium selenide, $NdSe$ | 5m | 71 |
| Magnesium tin, Mg_2Sn | 5 | 41 | Neodymium silver, $NdAg$ | 5m | 71 |
| Magnesium tin oxide, Mg_2SnO_4 | 10m | 37 | Neodymium vanadium oxide, $NdVO_4$ | 4m | 30 |
| Magnesium tungsten oxide, $MgWO_4$ | 1 | 84 | Neptunium nitride, NpN | 4m | 64 |
| Manganese, alpha, Mn | 7m | 142 | Nickel, Ni | 1 | 13 |
| Manganese aluminum oxide (galaxite), $MnAl_2O_4$ | 9 | 35 | Nickel aluminum, $NiAl$ | 6m | 82 |
| Manganese bromide, $MnBr_2$ | 4m | 63 | Nickel aluminum oxide, $NiAl_2O_4$ | 9 | 42 |
| Manganese(II) carbonate (rhodochrosite), $MnCO_3$ | 7 | 32 | Nickel arsenide 1:2 (rammelsbergite), $NiAs_2$ | 10 | 42 |
| Manganese chloride hydrate, $MnCl_2 \cdot 2H_2O$ | 11m | 38 | Nickel arsenic sulfide (gersdorffite), $NiAsS$ | 1m | 35 |
| Manganese chloride (scacchite), $MnCl_2$ | 8m | 43 | Nickel bromide, $NiBr$ | 10m | 119 |
| Manganese chloride hydrate, $MnCl_2 \cdot 4H_2O$ | 9m | 28 | Nickel(II) carbonate, $NiCO_3$ (trigonal)..... | 1m | 36 |
| Manganese cobalt oxide, $MnCo_2O_4$ | 9m | 30 | Nickel chloride, $NiCl_2$ | 9m | 81 |
| Manganese fluoride, MnF | 10m | 105 | Nickel chloride hydrate, $NiCl_2 \cdot 6H_2O$ | 11m | 42 |
| Manganese iodide, MnI_2 | 4m | 63 | Nickel fluoride, NiF | 10m | 121 |
| Manganese iron oxide (jacobsite), $MnFe_2O_4$... | 9 | 36 | Nickel fluoride hydrate, $NiF_2 \cdot 4H_2O$ | 11m | 43 |
| Manganese oxide (hausmannite), Mn_3O_4 | 10m | 38 | Nickel gallium oxide, $NiGa_2O_4$ | 10 | 45 |
| Manganese oxide (partridgeite), alpha Mn_2O_3 , (revised)..... | 11m | 95 | Nickel germanium oxide, Ni_2GeO_4 | 9 | 43 |
| Manganese oxide (pyrolusite), beta, MnO_2 | 10m | 39 | Nickel iron oxide (trevorite), $NiFe_2O_4$ | 10 | 44 |
| Manganese oxide hydroxide, groutite, alpha $MnOOH$ | 11m | 97 | Nickel(II) oxide (bunsenite), NiO | 1 | 47 |
| Manganese(II) oxide (manganosite), MnO | 5 | 45 | Nickel phosphide, $Ni_{12}P_5$ | 9m | 83 |
| Manganese selenide, $MnSe$ | 10 | 41 | Nickel silicon fluoride hydrate, $NiSiF_6 \cdot 6H_2O$ | 8 | 38 |
| Manganese sulfide (alabandite), alpha MnS | 4 | 11 | Nickel sulfate, $NiSO_4$ | 2m | 26 |
| Manganese(II) tungsten oxide (huebnerite), $MnWO_4$ | 2m | 24 | Nickel sulfate hydrate (retgersite), $NiSO_4 \cdot 6H_2O$ | 7 | 36 |
| Manganese vanadium oxide, $Mn_2V_2O_7$ | 9m | 75 | Nickel sulfide, millerite, NiS | 1m | 37 |
| Mercury amide chloride, $HgNH_2Cl$ | 10m | 40 | Nickel tungsten oxide, $NiWO_4$ | 2m | 27 |
| Mercury ammine chloride, $Hg(NH_3)_2Cl_2$ | 11m | 39 | Niobium gold 3:1, Nb_3Au | 6m | 16 |
| Mercury bromate, $Hg(BrO_3)_2$ | 10m | 107 | Niobium iridium 3:1, Nb_3Ir | 6m | 19 |
| Mercury bromide, $HgBr_2$ | 10m | 110 | Niobium osmium 3:1, Nb_3Os | 6m | 30 |
| Mercury(I) bromide, Hg_2Br_2 | 7 | 33 | Niobium oxychloride, $NbOC_1$ | 7m | 148 |
| Mercury(I) chloride (calomel), Hg_2Cl_2 | 1 | 72 | Niobium platinum 3:1, Nb_3Pt | 6m | 31 |
| Mercury(II) chloride, $HgCl_2$ | 1 | 73 | Niobium silicide, $NbSi_2$ | 8 | 39 |
| Mercury chloride sulfide, alpha $Hg_3Cl_2S_2$ | 8m | 118 | Osmium, Os | 4 | 8 |
| Mercury(II) cyanide, $Hg(CN)_2$ | 6 | 35 | Osmium titanium, $OsTi$ | 6m | 85 |
| Mercury(II) fluoride, HgF_2 | 2m | 25 | Palladium, Pd | 1 | 21 |
| Mercury(I) iodide, HgI | 4 | 49 | Palladium hydride, $PdH_{0.706}$ | 5m | 72 |
| Mercury iodide, HgI_2 (tetragonal) (revised) ... | 7m | 32 | Palladium oxide, PdO | 4 | 27 |
| Mercury(II) oxide (montroydite) HgO (revised) | 9 | 39 | Phosphorus bromide, PBr | 7m | 150 |
| Mercury(II) selenide (tiemannite), $HgSe$ | 7 | 35 | Phosphorus oxide (stable form I), P_2O_5 , (orthorhombic) | 9m | 86 |
| Mercury(II) sulfide (cinnabar), HgS (hex- agonal) | 4 | 17 | Phosphorus oxide (stable form II), P_2O_5 , (orthorhombic) | 9m | 88 |
| Mercury(II) sulfide (metacinnabar), HgS (cubic) | 4 | 21 | Phosphorus oxide (metastable form), P_4O_{10} , (rhombohedral) | 9m | 91 |
| Molybdenum, Mo | 1 | 20 | Platinum, Pt | 1 | 31 |
| Molybdenum arsenide, Mo_3As | 10m | 115 | Platinum titanium 1:3, $PtTi_3$ | 6m | 33 |
| Molybdenum osmium 3:1, Mo_3Os | 6m | 28 | Plutonium arsenide, $PuAs$ | 4m | 65 |
| | | | Plutonium phosphide, PuP | 4m | 65 |
| | | | Plutonium telluride, $PuTe$ | 4m | 66 |
| | | | Potassium aluminum sulfate hydrate, (alum), $KAl(SO_4)_2 \cdot 12H_2O$ | 9m | 31 |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|--|-----------------|------|
| Potassium barium nickel nitrite, $K_2BaNi(NO_3)_4$ | 9m | 32 | Potassium molybdenum oxide phosphate hydrate, $K_2(MoO_3)_{12}PO_4 \cdot 4H_2O$ | 8 | 43 |
| Potassium borohydride, KBH_4 | 9 | 44 | Potassium nickel fluoride, $KNiF_3$ | 7m | 42 |
| Potassium bromate, $KBrO_3$ | 7 | 38 | Potassium nickel fluoride, K_2NiF_4 | 10m | 45 |
| Potassium bromide, KBr | 1 | 66 | Potassium nickel (II) sulfate, $K_2Ni_2(SO_4)_3$ | 6m | 46 |
| Potassium bromide chloride, $KBr_{0.5}Cl_{0.5}$ | 8m | 46 | Potassium niobium fluoride, K_2NbF_6 | 8m | 120 |
| Potassium bromide iodide, $KBr_{0.33}I_{0.67}$ | 11m | 44 | Potassium nitrate (niter), KNO_3 | 3 | 58 |
| Potassium bromide iodide, $KBr_{0.67}I_{0.33}$ | 11m | 45 | Potassium nitrite, KNO_2 | 9m | 38 |
| Potassium cadmium fluoride, $KCdF_3$ | 8m | 47 | Potassium nitroso ruthenium chloride, $K_2(NO)RuCl_5$ | 2m | 29 |
| Potassium cadmium sulfate, $K_2Cd(SO_4)_2$ | 7m | 34 | Potassium oxide, K_2O | 10m | 125 |
| Potassium calcium carbonate (fairchildite), $K_2Ca(CO_3)_2$ | 8m | 48 | Potassium platinum bromide, K_2PtBr_6 | 8 | 40 |
| Potassium calcium chloride (chlorocalcite), $KCaCl_3$ | 7m | 36 | Potassium platinum chloride, K_2PtCl_6 | 5 | 49 |
| Potassium calcium fluoride, $KCaF_3$ | 8m | 49 | Potassium platinum fluoride, K_2PtF_6 | 6 | 42 |
| Potassium calcium magnesium sulfate, $K_2CaMg(SO_4)_3$ | 7m | 37 | Potassium rhenium chloride, K_2ReCl_6 | 2m | 28 |
| Potassium calcium nickel nitrite, $K_2CaNi(NO_2)_6$ | 9m | 33 | Potassium rhodium oxide, $KReO_4$ | 8 | 41 |
| Potassium calcium sulfate, $K_2Ca_2(SO_4)_3$ | 7m | 39 | Potassium rubidium chloride, $Rb_{0.5}K_{0.5}Cl$ | 8m | 76 |
| Potassium chlorate, $KClO_3$ | 3m | 42 | Potassium ruthenium chloride, K_2RuCl_6 | 10 | 46 |
| Potassium chlorate, $KClO_4$ | 6 | 43 | Potassium ruthenium oxide chloride hydrate, $K_4Ru_2OCl_{10} \cdot H_2O$ | 10 | 47 |
| Potassium chloride (sylvite), KCl | 1 | 65 | Potassium selenate, K_2SeO_4 | 9m | 41 |
| Potassium chromium oxide, K_2CrO_4 | 3m | 44 | Potassium selenide, K_2Se | 10m | 126 |
| Potassium chromium sulfate hydrate, $KCr(SO_4)_2 \cdot 12H_2O$ | 6 | 39 | Potassium selenium bromide, K_2SeBr_6 | 8 | 41 |
| Potassium cobalt(II) fluoride, $KCoF_3$ | 6m | 37 | Potassium silicon fluoride (hieratite), K_2SiF_6 | 5 | 50 |
| Potassium cobalt fluoride, K_2CoF_4 | 11m | 46 | Potassium silver cyanide, $KAg(CN)_2$ | 8m | 78 |
| Potassium cobalt nitrite, $K_3Co(NO_2)_6$ | 9 | 45 | Potassium sodium aluminum fluoride (elpasolite), K_2NaAlF_6 | 9m | 43 |
| Potassium cobalt (II) sulfate, $K_2Co_2(SO_4)_3$ | 6m | 35 | Potassium sodium sulfate, $KNaSO_4$ | 6m | 50 |
| Potassium copper chloride, $KCuCl_3$ | 7m | 41 | Potassium sodium sulfate (aphthitalite), $K_3Na(SO_4)_2$ | 6m | 48 |
| Potassium copper chloride hydrate (mitscherlichite), $K_2CuCl_4 \cdot 2H_2O$ | 9m | 34 | Potassium sulfate, $K_2S_2O_7$ | 9m | 52 |
| Potassium copper(II) fluoride, $KCuF_3$ | 6m | 38 | Potassium sulfate (arcanite), K_2SO_4 | 3 | 62 |
| Potassium cyanate, $KCNO$ | 7 | 39 | Potassium sulfide, K_2S | 10m | 127 |
| Potassium cyanide, KCN | 1 | 77 | Potassium telluride, K_2Te | 10m | 128 |
| Potassium fluoride, KF | 1 | 64 | Potassium thiocyanate, $KCNS$ | 8 | 44 |
| Potassium germanium fluoride, K_2GeF_6 | 6 | 41 | Potassium tin chloride, K_2SnCl_6 | 6 | 38 |
| Potassium hydrogen arsenate, KH_2AsO_4 | 1m | 38 | Potassium titanium fluoride, K_2TiF_6 | 7 | 40 |
| Potassium hydrogen phosphate, KH_2PO_4 | 3 | 69 | Potassium tungsten oxide, K_2WO_4 | 11m | 47 |
| Potassium hydroxide, KOH at 300 °C | 4m | 66 | Potassium vanadium oxide, KV_3O_8 | 8m | 56 |
| Potassium iodide, KI | 1 | 68 | Potassium zinc bromide hydrate, $KZnBr_2 \cdot 2H_2O$ | 11m | 104 |
| Potassium iodate, KIO_4 | 7 | 41 | Potassium zinc fluoride, $KZnF_3$ | 5 | 51 |
| Potassium iron cyanide, $K_3Fe(CN)_6$ | 9m | 35 | Potassium zinc fluoride, K_2ZnF_4 | 10m | 46 |
| Potassium iron fluoride, K_3FeF_6 | 9m | 37 | Potassium zinc iodide hydrate, $KZnI_3 \cdot 2H_2O$ | 11m | 107 |
| Potassium iron(II) fluoride, $KFeF_3$ | 6m | 39 | Potassium zinc sulfate, $K_2Zn_2(SO_4)_3$ | 6m | 54 |
| Potassium lithium sulfate, $KLiSO_4$ | 3m | 43 | Potassium zinc sulfate hydrate, $K_2Zn(SO_4)_2 \cdot 6H_2O$ | 7m | 43 |
| Potassium magnesium chloride hydrate (carnallite), $KMgCl_3 \cdot 6H_2O$ | 8m | 50 | Potassium zinc vanadium oxide hydrate, $K_2Zn_2V_{10}O_{28} \cdot 16H_2O$ | 3m | 45 |
| Potassium magnesium chromium oxide, $K_2Mg_2(CrO_4)_3$ | 8m | 52 | Potassium zirconium fluoride, K_2ZrF_7 | 9 | 46 |
| Potassium magnesium fluoride, $KMgF_3$ | 6m | 42 | Praseodymium antimony, $PrSb$ | 4m | 43 |
| Potassium magnesium fluoride, K_2MgF_4 | 10m | 42 | Praseodymium arsenate, $PrAsO_4$ | 4m | 32 |
| Potassium magnesium selenate hydrate, $K_2Mg(SeO_4)_2 \cdot 6H_2O$ | 10m | 43 | Praseodymium arsenide, $PrAs$ | 4m | 67 |
| Potassium magnesium sulfate (langbeinite), $K_2Mg_2(SO_4)_3$ | 6m | 40 | Praseodymium bismuth, $PrBi$ | 4m | 49 |
| Potassium magnesium sulfate hydrate (picromerite), $K_2Mg(SO_4)_2 \cdot 6H_2O$ | 8m | 54 | Praseodymium cadmium, $PrCd$ | 5m | 64 |
| Potassium manganese (II) fluoride, $KMnF_3$ | 6m | 45 | Praseodymium chloride, $PrCl_3$ | 1m | 39 |
| Potassium manganese oxide, $KMnO_4$ | 7 | 42 | Praseodymium fluoride, PrF_3 | 5 | 52 |
| Potassium manganese (II) sulfate (manganolangbeinite), $K_2Mn_2(SO_4)_3$ | 6m | 43 | Praseodymium oxychloride, $PrOCl$ | 9 | 47 |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|--|-----------------|------|
| Rubidium amide, RbNH ₂ | 5m | 73 | Samarium oxychloride, SmOCl | 1m | 43 |
| Rubidium bromate, RbBrO ₃ | 8 | 45 | Samarium silver, SmAg | 5m | 73 |
| Rubidium bromide, RbBr | 7 | 43 | Samarium tin oxide, Sm ₂ Sn ₂ O ₇ | 8m | 77 |
| Rubidium cadmium chloride, high form, RbCdCl ₃ (tetragonal) | 5m | 43 | Samarium vanadium oxide, SmVO ₄ | 5m | 47 |
| Rubidium cadmium chloride, low form, RbCdCl ₃ (orthorhombic) | 5m | 41 | Scandium antimony, ScSb | 4m | 44 |
| Rubidium cadmium sulfate, Rb ₂ Cd ₂ (SO ₄) ₃ | 7m | 45 | Scandium arsenate, ScAsO ₄ | 4m | 35 |
| Rubidium calcium chloride, RbCaCl ₃ | 7m | 47 | Scandium arsenide, ScAs | 4m | 68 |
| Rubidium calcium fluoride, RbCaF ₃ | 8m | 57 | Scandium oxide, Sc ₂ O ₃ | 3 | 27 |
| Rubidium calcium sulfate, Rb ₂ Ca ₂ (SO ₄) ₃ | 7m | 48 | Scandium phosphate, ScPO ₄ | 8 | 50 |
| Rubidium chlorate, RbClO ₃ | 8 | 47 | Scandium silicate (thortveitite), Sc ₂ Si ₂ O ₇ | 7m | 58 |
| Rubidium chlorate, RbClO ₄ | 2m | 30 | Selenium, Se | 5 | 54 |
| Rubidium chloride, RbCl | 4 | 41 | Selenium oxide (selenolite), SeO ₂ , (revised). | 7m | 60 |
| Rubidium chromium oxide, Rb ₂ CrO ₄ | 3m | 46 | Silicon, Si | 2 | 6 |
| Rubidium chromium sulfate hydrate, RbCr(SO ₄) ₂ ·12H ₂ O | 6 | 47 | Silicon oxide, (alpha or low cristobalite), SiO ₂ (tetragonal) (revised) | 10 | 48 |
| Rubidium cobalt (II) chloride, RbCoCl ₃ | 6m | 57 | Silicon oxide (alpha or low quartz), SiO ₂ (hexagonal) | 3 | 24 |
| Rubidium cobalt fluoride, RbCoF ₃ | 8m | 58 | Silicon oxide (beta or high cristobalite), SiO ₂ (cubic) | 1 | 42 |
| Rubidium cobalt sulfate, Rb ₂ Co ₂ (SO ₄) ₃ | 8m | 59 | Silver, Ag | 1 | 23 |
| Rubidium copper chloride hydrate, Rb ₂ CuCl ₄ ·2H ₂ O | 10m | 47 | Silver, Ag (reference standard) | 8m | 2 |
| Rubidium copper sulfate hydrate, Rb ₂ Cu(SO ₄) ₂ ·6H ₂ O | 8m | 61 | Silver antimony sulfide, AgSbS ₂ (cubic) | 5m | 48 |
| Rubidium fluoride, RbF | 8m | 63 | Silver antimony sulfide (miargyrite), AgSbS ₂ (monoclinic) | 5m | 49 |
| Rubidium iodate, RbIO ₄ | 2m | 31 | Silver antimony sulfide (pyrargyrite), Ag ₃ SbS ₃ (trigonal) | 5m | 51 |
| Rubidium iodide, RbI | 4 | 43 | Silver antimony telluride, AgSbTe ₂ | 3m | 47 |
| Rubidium iron sulfate hydrate, Rb ₂ Fe(SO ₄) ₂ ·6H ₂ O | 8m | 64 | Silver arsenate, Ag ₃ AsO ₄ | 5 | 56 |
| Rubidium magnesium chromium oxide, Rb ₂ Mg ₂ (CrO ₄) ₃ | 8m | 66 | Silver arsenic sulfide, xanthoconite, Ag ₃ AsS ₃ | 8m | 126 |
| Rubidium magnesium chromium oxide hydrate, Rb ₂ Mg(CrO ₄) ₂ ·6H ₂ O | 8m | 68 | Silver bromate, AgBrO | 5 | 57 |
| Rubidium magnesium sulfate, Rb ₂ Mg ₂ (SO ₄) ₃ | 7m | 50 | Silver bromide (bromyrite), AgBr | 4 | 46 |
| Rubidium magnesium sulfate hydrate, Rb ₂ Mg(SO ₄) ₂ ·6H ₂ O | 8m | 70 | Silver carbonate, Ag ₂ CO ₃ | 1m | 44 |
| Rubidium manganese (II) fluoride, RbMnF ₃ | 5m | 44 | Silver chlorate, AgClO ₃ | 7 | 44 |
| Rubidium manganese sulfate, Rb ₂ Mn ₂ (SO ₄) ₃ | 7m | 52 | Silver chloride, (cerargyrite), AgCl | 4 | 44 |
| Rubidium nickel (II) chloride, RbNiCl ₃ | 6m | 58 | Silver cyanide, AgCN | 9m | 48 |
| Rubidium nickel sulfate, Rb ₂ Ni ₂ (SO ₄) ₃ | 8m | 72 | Silver fluoride, Ag ₂ F | 5m | 53 |
| Rubidium nickel sulfate hydrate, Rb ₂ Ni(SO ₄) ₂ ·6H ₂ O | 8m | 74 | Silver iodate, AgIO ₄ | 9 | 49 |
| Rubidium nitrate, RbNO ₃ (trigonal) | 5m | 45 | Silver iodide (iodyrite), AgI (hexagonal) | 8 | 51 |
| Rubidium platinum chloride, Rb ₂ PtCl ₆ | 5 | 53 | Silver iodide, gamma, AgI (cubic) | 9 | 48 |
| Rubidium platinum fluoride, Rb ₂ PtF ₆ | 6 | 48 | Silver manganese oxide, AgMnO ₄ | 7m | 155 |
| Rubidium selenate, Rb ₂ SeO ₄ | 9m | 44 | Silver molybdenum oxide, Ag ₂ MoO ₄ | 7 | 45 |
| Rubidium silicon fluoride, Rb ₂ SiF ₆ | 6 | 49 | Silver nitrate, AgNO ₃ | 5 | 59 |
| Rubidium strontium chloride, RbSrCl ₃ | 7m | 54 | Silver nitrite, AgNO ₂ | 5 | 60 |
| Rubidium sulfate, Rb ₂ SO ₄ | 8 | 48 | Silver oxide, Ag ₂ O | 1m | 45 |
| Rubidium tellurium bromide, Rb ₂ TeBr ₆ | 8 | 46 | Silver(II) oxide nitrate, Ag ₂ O ₂ NO ₃ | 4 | 61 |
| Rubidium tellurium chloride, Rb ₂ TeCl ₆ | 8 | 48 | Silver phosphate, Ag ₃ PO ₄ | 5 | 62 |
| Rubidium tin chloride, Rb ₂ SnCl ₆ | 6 | 46 | Silver rhenium oxide, AgReO ₄ | 8 | 53 |
| Rubidium zinc fluoride, RbZnF ₃ | 7m | 57 | Silver selenate, Ag ₂ SeO ₄ | 2m | 32 |
| Rubidium zinc sulfate hydrate, Rb ₂ Zn(SO ₄) ₂ ·6H ₂ O | 7m | 55 | Silver sodium chloride, Ag _{0.5} Na _{0.5} Cl | 8m | 79 |
| Ruthenium, Ru | 4 | 5 | Silver sulfate, Ag ₂ SO ₄ | 7 | 46 |
| Ruthenium titanium, RuTi | 6m | 86 | Silver sulfide (argentite), Ag ₂ S | 10 | 51 |
| Samarium arsenate, SmAsO ₄ | 4m | 33 | Sodium, Na | 9m | 105 |
| Samarium arsenide, SmAs | 4m | 68 | Sodium aluminum chloride silicate, sodalite, Na ₈ Al ₆ Cl ₂ (SiO ₄) ₆ | 7m | 158 |
| Samarium chloride, SmCl ₃ | 1m | 40 | Sodium azide, alpha, NaN ₃ , at -90 to -100°C | 8m | 129 |
| Samarium fluoride, SmF ₃ | 1m | 41 | Sodium azide, beta NaN ₃ | 8m | 130 |
| Samarium gallium oxide, Sm ₃ Ga ₂ (GaO ₄) ₃ | 1m | 42 | Sodium beryllium calcium fluoride silicate, leucophanite, NaBeCaFSi ₂ O ₆ | 8m | 138 |
| Samarium oxide, Sm ₂ O ₃ (cubic) | 4m | 34 | Sodium borate, Na ₂ B ₄ O ₇ | 7m | 160 |
| M—Monograph 25. | | | Sodium boron hydride, NaBH ₄ | 9 | 51 |
| A mineral name in () indicates a synthetic sample. | | | Sodium bromate, NaBrO ₃ | 5 | 65 |
| | | | Sodium bromide, NaBr | 3 | 47 |
| | | | Sodium bromide chloride, NaBr _{0.33} Cl _{0.67} | 11m | 49 |
| | | | Sodium bromide chloride, NaBr _{0.67} Cl _{0.33} | 11m | 50 |
| | | | Sodium calcium aluminum fluoride hydrate, thomsonelite, NaCaAlF ₆ ·H ₂ O | 8m | 132 |

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|--|-----------------|------|
| Sodium calcium beryllium aluminum fluorosilicate, meliphanite, $(\text{Na}_{0.6}\text{Ca}_{1.3})\text{Be}(\text{Al}_{0.13}\text{Si}_{1.87})$ $(\text{O}_{6.25}\text{F}_{0.75})$ | 8m | 135 | Sodium nitrite, NaNO_2 | 4 | 62 |
| Sodium calcium carbonate hydrate, pirssonite, $\text{Na}_2\text{Ca}(\text{CO}_3)_2 \cdot 2\text{H}_2\text{O}$ | 9m | 106 | Sodium oxide, Na_2O | 10m | 134 |
| Sodium calcium silicate, $\text{Na}_2\text{CaSiO}_4$ | 10m | 48 | Sodium phosphate, $\text{Na}_3\text{P}_2\text{O}_7$ | 3m | 49 |
| Sodium calcium sulfate (glauberite), $\text{Na}_2\text{Ca}(\text{SO}_4)_2$ | 6m | 59 | Sodium phosphate hydrate, $\text{Na}_3\text{P}_2\text{O}_7 \cdot \text{H}_2\text{O}$ | 3m | 50 |
| Sodium carbonate hydrate (thermonatrite), $\text{Na}_2\text{CO}_3 \cdot \text{H}_2\text{O}$ | 8 | 54 | Sodium phosphate hydrate, alpha $\text{Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (monoclinic) | 10 | 52 |
| Sodium carbonate sulfate, $\text{Na}_4\text{CO}_3\text{SO}_4$ | 11m | 51 | Sodium phosphate hydrate, beta $\text{Na}_4\text{P}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$ (triclinic) | 2m | 35 |
| Sodium carbonate sulfate (burkeite), $\text{Na}_4\text{CO}_3(\text{SO}_4)_2$ | 11m | 52 | Sodium phosphate hydrate, $\text{Na}_6\text{P}_6\text{O}_{18} \cdot 6\text{H}_2\text{O}$ | 5m | 54 |
| Sodium carbonate sulfate, $\text{Na}_6\text{CO}_3(\text{SO}_4)_2$ | 11m | 53 | Sodium praseodymium fluoride silicate, $(\text{Na}_2\text{Pr}_6)\text{F}_2(\text{SiO}_4)_6$ | 7m | 68 |
| Sodium carbonate sulfate, $\text{Na}_6(\text{CO}_3)_2\text{SO}_4$ | 11m | 54 | Sodium selenate, Na_2SeO_4 | 9m | 55 |
| Sodium chlorate, NaClO_3 | 3 | 51 | Sodium selenide, Na_2Se | 10m | 135 |
| Sodium chlorate, NaClO_3 , orthorhombic | 7 | 49 | Sodium silicate, alpha (III), $\text{Na}_2\text{Si}_2\text{O}_5$ | 8m | 141 |
| Sodium chloride (halite), NaCl | 2 | 41 | Sodium silicate, beta $\text{Na}_2\text{Si}_2\text{O}_5$ | 10m | 136 |
| Sodium chromium oxide, Na_2CrO_4 | 9m | 48 | Sodium sulfate (thenardite), Na_2SO_4 | 2 | 59 |
| Sodium chromium oxide hydrate, $\text{Na}_2\text{Cr}_2\text{O}_7 \cdot 2\text{H}_2\text{O}$ | 7m | 62 | Sodium sulfate, Na_2SO_4 | 11m | 57 |
| Sodium chromium oxide hydrate, $\text{Na}_2\text{CrO}_4 \cdot 4\text{H}_2\text{O}$ | 9m | 50 | Sodium sulfide, Na_2S | 10m | 140 |
| Sodium chromium oxide sulfate, $\text{Na}_4(\text{CrO}_4)(\text{SO}_4)$ | 11m | 55 | Sodium sulfite, Na_2SO_3 | 3 | 60 |
| Sodium cobalt(II) sulfate hydrate, $\text{Na}_2\text{Co}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 61 | Sodium telluride, Na_2Te | 10m | 141 |
| Sodium cyanate, NaCNO | 2m | 33 | Sodium tin fluoride, NaSn_3F_6 | 7m | 166 |
| Sodium cyanide, NaCN (cubic) | 1 | 78 | Sodium tungsten oxide, Na_2WO_4 | 1m | 47 |
| Sodium cyanide, NaCN (orthorhombic) at 6 °C | 1 | 79 | Sodium tungsten(VI) oxide hydrate, $\text{Na}_2\text{WO}_4 \cdot 2\text{H}_2\text{O}$ | 2m | 33 |
| Sodium fluoride (villiaumite), NaF | 1 | 63 | Sodium zinc fluoride, NaZnF_3 | 6m | 74 |
| Sodium hydrogen fluoride, NaHF_2 | 5 | 63 | Sodium zinc sulfate hydrate, $\text{Na}_2\text{Zn}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 72 |
| Sodium hydrogen phosphate, $\text{Na}_3\text{H}(\text{PO}_4)_2$ | 10m | 130 | Sodium zirconium fluoride, $\text{Na}_2\text{Zr}_6\text{F}_{31}$ | 8m | 144 |
| Sodium hydrogen silicate hydrate, $\text{Na}_2\text{H}_2\text{SiO}_4 \cdot 4\text{H}_2\text{O}$ | 7m | 163 | Strontium aluminum hydroxide, $\text{Sr}_3\text{Al}_2(\text{OH})_1$ | 10m | 50 |
| Sodium hydrogen sulfate hydrate, $\text{NaHSO}_4 \cdot \text{H}_2\text{O}$ | 9m | 52 | Strontium aluminum oxide, $\text{Sr}_3\text{Al}_2\text{O}_6$ | 10m | 52 |
| Sodium hydroxide, NaOH at 300 °C | 4m | 69 | Strontium arsenate, $\text{Sr}_3(\text{AsO}_4)_2$ | 2m | 36 |
| Sodium iodate, NaIO_3 | 7 | 47 | Strontium azide, $\text{Sr}(\text{N}_3)_2$ | 8m | 146 |
| Sodium iodate, NaIO_4 | 7 | 48 | Strontium borate, SrB_2O_4 | 3m | 53 |
| Sodium iodide, NaI | 4 | 31 | Strontium borate, SrB_4O_7 | 4m | 36 |
| Sodium iron fluoride, Na_3FeF_6 | 9m | 54 | Strontium bromide fluoride, SrBrF | 10m | 54 |
| Sodium lanthanum fluoride silicate, $(\text{Na}_2\text{La}_3)\text{F}_2(\text{SiO}_4)_6$ | 7m | 64 | Strontium bromide hydrate, $\text{SrBr}_2 \cdot 6\text{H}_2\text{O}$ | 4 | 60 |
| Sodium lanthanum molybdenum oxide, $\text{NaLa}(\text{MoO}_4)_2$ | 10m | 49 | Strontium carbonate (strontianite), SrCO_3 | 3 | 56 |
| Sodium magnesium aluminum boron hydroxide silicate, dravite, $\text{NaMg}_2\text{Al}_2\text{B}_3(\text{OH})_4\text{Si}_8\text{O}_{27}$ | 3m | 47 | Strontium chloride, SrCl_2 | 4 | 40 |
| Sodium magnesium carbonate (eitelite), $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ | 11m | 56 | Strontium chloride fluoride, SrClF | 10m | 55 |
| Sodium magnesium sulfate hydrate, bloedite, $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 63 | Strontium chloride hydrate, $\text{SrCl}_2 \cdot 6\text{H}_2\text{O}$ | 4 | 58 |
| Sodium manganese(II) fluoride, NaMnF_3 | 6m | 65 | Strontium chloride hydrate, $\text{SrCl}_2 \cdot 2\text{H}_2\text{O}$ | 11m | 58 |
| Sodium mercury (II) chloride hydrate, $\text{NaHgCl}_2 \cdot 2\text{H}_2\text{O}$ | 6m | 66 | Strontium chloride hydroxide phosphate, $\text{Sr}_5\text{Cl}_{1.66}\text{OH}_{1.15}(\text{PO}_4)_3$ | 11m | 60 |
| Sodium molybdenum oxide, Na_2MoO_4 | 1m | 46 | Strontium fluoride, SrF_2 | 5 | 67 |
| Sodium molybdenum oxide, $\text{Na}_2\text{Mo}_2\text{O}_7$ | 9m | 110 | Strontium indium hydroxide, $\text{Sr}_3\text{In}_2(\text{OH})_{12}$ | 6m | 76 |
| Sodium neodymium fluoride silicate, $(\text{Na}_2\text{Nd}_3)\text{F}_2(\text{SiO}_4)_6$ | 7m | 66 | Strontium iodide hydrate, $\text{SrI}_2 \cdot 6\text{H}_2\text{O}$ | 8 | 58 |
| Sodium nickel (II) sulfate hydrate, $\text{Na}_2\text{Ni}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 68 | Strontium manganese oxide, SrMnO_3 (cubic) | 10m | 56 |
| Sodium nitrate (soda-niter), NaNO_3 | 6 | 50 | Strontium manganese oxide, SrMnO_3 (hexagonal) | 10m | 58 |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|--|-----------------|------|---|-----------------|------|
| Sulfur, S (orthorhombic) | 9 | 54 | Thorium antimony, ThSb | 4m | 44 |
| Tantalum, Ta | 1 | 29 | Thorium arsenide, ThAs | 4m | 70 |
| Tantalum silicide, TaSi ₂ | 8 | 59 | Thorium oxide (thorianite), ThO ₂ | 1 | 57 |
| Tellurium, Te | 1 | 26 | Thulium antimony, TmSb | 4m | 45 |
| Tellurium(IV) oxide (paratellurite), TeO ₂ , (tetragonal) | 7 | 56 | Thulium arsenate, TmAsO ₄ | 3m | 56 |
| Tellurium(IV) oxide, paratellurite, TeO ₂ , (tetragonal) | 10 | 55 | Thulium arsenide, TmAs | 4m | 71 |
| Tellurium(IV) oxide, tellurite, TeO ₂ (orthorhombic) | 9 | 57 | Thulium nitride, TmN | 4m | 71 |
| Terbium antimony, TbSb | 5m | 61 | Thulium oxide, Tm ₂ O ₃ | 9 | 58 |
| Terbium arsenate, TbAsO ₄ | 3m | 54 | Thulium silver, TmAg | 5m | 74 |
| Terbium arsenide, TbAs | 5m | 75 | Thulium telluride, TmTe | 4m | 72 |
| Terbium nitride, TbN | 4m | 70 | Thulium vanadium oxide, TmVO ₄ | 5m | 57 |
| Terbium phosphide, TbP | 5m | 76 | Tin, alpha Sn (cubic) | 2 | 12 |
| Terbium selenide, TbSe | 5m | 76 | Tin, arsenide, SnAs | 4m | 37 |
| Terbium silver, TbAg | 5m | 74 | Tin, beta Sn (tetragonal) | 1 | 24 |
| Terbium sulfide, TbS | 5m | 77 | Tin(II) fluoride, SnF ₂ | 3m | 51 |
| Terbium telluride, TbTe | 5m | 77 | Tin(IV) iodide, SnI ₄ | 5 | 71 |
| Terbium vanadium oxide, TbVO ₄ | 5m | 56 | Tin(II) oxide, SnO | 4 | 28 |
| Thallium aluminum sulfate hydrate, TlAl(SO ₄) ₂ ·12H ₂ O | 6 | 53 | Tin(IV) oxide (cassiterite), SnO ₂ | 1 | 54 |
| Thallium(I) arsenate, Tl ₁ AsO ₄ | 2m | 37 | Tin sulfide (berndtite), beta SnS ₂ | 9m | 57 |
| Thallium azide, TlN _x | 8m | 82 | Tin(II) telluride, SnTe | 7 | 61 |
| Thallium(I) bromate, TlBrO ₃ | 8 | 60 | Titanium, Ti | 3 | 1 |
| Thallium bromide, TlBr | 7 | 57 | Titanium oxide (anatase), TiO _x (revised) | 7m | 82 |
| Thallium cadmium sulfate, Tl ₂ Cd ₂ (SO ₄) ₃ | 8m | 83 | Titanium oxide, brookite, TiO ₂ (orthorhombic) | 3m | 57 |
| Thallium (I) chlorate, TlClO ₄ | 2m | 38 | Titanium oxide (rutile), TiO _x (revised) | 7m | 83 |
| Thallium(I) chloride, TlClO ₃ | 8 | 61 | Titanium(III) oxide, TiO _{1.515} | 9 | 59 |
| Thallium(I) chloride, TlCl | 4 | 51 | Titanium silicide, Ti ₅ Si ₃ | 8 | 64 |
| Thallium chromium oxide, Tl ₂ CrO ₄ | 3m | 54 | Titanium sulfide, TiS ₂ | 4m | 72 |
| Thallium chromium sulfate hydrate, TlCr(SO ₄) ₂ ·12H ₂ O | 6 | 55 | Titanium sulfide, Ti ₂ S | 8m | 149 |
| Thallium cobalt sulfate, Tl ₂ Co ₂ (SO ₄) ₃ | 8m | 85 | Tungsten, W | 1 | 28 |
| Thallium cobalt sulfate hydrate, Tl ₂ Co(SO ₄) ₂ ·6H ₂ O | 7m | 70 | Tungsten, W (reference standard) | 8m | 2 |
| Thallium copper sulfate hydrate, Tl ₂ Cu(SO ₄) ₂ ·6H ₂ O | 7m | 72 | Tungsten sulfide (tungstenite), WS ₂ | 8 | 65 |
| Thallium gallium sulfate hydrate, TlGa(SO ₄) ₂ ·12H ₂ O | 6 | 57 | Uranium oxide, UO | 5m | 78 |
| Thallium(I) iodate, TlIO ₃ | 8 | 62 | Uranium oxide (uraninite), UO ₂ | 2 | 33 |
| Thallium(I) iodide, TlI (orthorhombic) | 4 | 53 | Uranium selenide, USe | 5m | 78 |
| Thallium iron sulfate hydrate, Tl ₂ Fe(SO ₄) ₂ ·6H ₂ O | 8m | 87 | Uranium telluride, UTe | 4m | 73 |
| Thallium magnesium chromium oxide, Tl ₂ Mg ₂ (CrO ₄) ₃ | 8m | 89 | Vanadium, V | 9m | 58 |
| Thallium manganese sulfate, Tl ₂ Mn ₂ (SO ₄) ₃ | 7m | 76 | Vanadium gold 3:1, V ₃ Au | 6m | 18 |
| Thallium magnesium sulfate hydrate, Tl ₂ Mg(SO ₄) ₂ ·6H ₂ O | 7m | 74 | Vanadium iridium 3:1, V ₃ Ir | 6m | 21 |
| Thallium nickel sulfate hydrate, Tl ₂ Ni(SO ₄) ₂ ·6H ₂ O | 7m | 78 | Vanadium(V) oxide, V ₂ O ₅ | 8 | 66 |
| Thallium(I) nitrate, TlNO ₃ | 6 | 58 | Vanadium palladium 3:1, V ₃ Pd | 6m | 32 |
| Thallium(III) oxide, Tl ₂ O ₃ | 2 | 28 | Vanadium platinum 3:1, V ₃ Pt | 6m | 34 |
| Thallium(I) phosphate, Tl ₂ PO ₄ | 7 | 58 | Vanadium rhodium 3:1, V ₃ Rh | 6m | 56 |
| Thallium(III) phosphate, TlPO ₄ | 7 | 59 | Ytterbium antimony, YbSb | 4m | 45 |
| Thallium platinum chloride Tl ₂ PtCl ₆ | 5 | 70 | Ytterbium arsenate, YbAsO ₄ | 4m | 38 |
| Thallium silicon fluoride, Tl ₂ SiF ₆ | 6 | 56 | Ytterbium arsenide, YbAs | 4m | 73 |
| Thallium(I) sulfate, Tl ₂ SO ₄ | 6 | 59 | Ytterbium gallium oxide, Yb ₂ Ga ₃ (GaO ₄) ₃ | 1m | 49 |
| Thallium(I) thiocyanate, TlCNS | 8 | 63 | Ytterbium nitride, YbN | 4m | 74 |
| Thallium tin chloride, Tl ₂ SnCl ₆ | 6 | 54 | Ytterbium oxide, Yb ₂ O ₃ | 6m | 80 |
| Thallium(I) tungsten oxide, Tl ₂ WO ₄ | 1m | 48 | Ytterbium selenide, YbSe | 5m | 79 |
| Thallium zinc sulfate hydrate, Tl ₂ Zn(SO ₄) ₂ ·6H ₂ O | 7m | 80 | Ytterbium telluride, YbTe | 5m | 79 |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE INORGANIC INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|--|-----------------|------|--|-----------------|------|
| Zinc aluminum oxide (gahnite), ZnAl_2O_4 | 2 | 38 | Zinc selenide, ZnSe | 3 | 23 |
| Zinc ammine bromide, $\text{Zn}(\text{NH}_3)_2\text{Br}_2$ | 11m | 68 | Zinc silicate (willemite), Zn_2SiO_4 | 7 | 62 |
| Zinc ammine chloride, $\text{Zn}(\text{NH}_3)_2\text{Cl}_2$ | 10m | 59 | Zinc silicon fluoride hydrate, $\text{ZnSiF}_6 \cdot 6\text{H}_2\text{O}$.. | 8 | 70 |
| Zinc antimony oxide, ZnSb_2O_4 | 4m | 39 | Zinc sulfate (zinkosite), ZnSO_4 | 7 | 64 |
| Zinc borate, ZnB_2O_4 | 1 | 83 | Zinc sulfate hydrate (gossarite), $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$ | 8 | 71 |
| Zinc carbonate, smithsonite, ZnCO_3 , | 8 | 69 | Zinc sulfide (wurtzite), alpha ZnS (hexagonal) | 2 | 14 |
| Zinc chromium oxide, ZnCr_2O_4 | 9m | 59 | Zinc sulfide (sphalerite), beta ZnS (cubic) ... | 2 | 16 |
| Zinc cobalt oxide, ZnCo_2O_4 | 10m | 60 | Zinc telluride, ZnTe | 3m | 58 |
| Zinc cyanide, $\text{Zn}(\text{CN})_2$, | 5 | 73 | Zinc tin oxide, Zn_2SnO_4 | 10m | 62 |
| Zinc fluoride, ZnF_2 | 6 | 60 | Zinc tungsten oxide (sanmartinite), ZnWO_4 .. | 2m | 40 |
| Zinc fluoride hydrate, $\text{ZnF}_2 \cdot 4\text{H}_2\text{O}$ | 11m | 69 | Zirconium, alpha, Zr | 2 | 11 |
| Zinc germanium oxide, Zn_2GeO_4 | 10 | 56 | Zirconium hydride, ZrH_2 | 5m | 60 |
| Zinc hydroxide silicate hydrate, hemimorphite, $\text{Zn}_4(\text{OH})_2\text{Si}_2\text{O}_7 \cdot \text{H}_2\text{O}$ | 2 | 62 | Zirconium iodate, $\text{Zr}(\text{IO}_3)_4$ | 1m | 51 |
| Zinc iodide, ZnI_2 | 9 | 60 | Zirconium nitride, ZrN | 5m | 80 |
| Zinc iron oxide (franklinite), ZnFe_2O_4 | 9m | 60 | Zirconium oxide, ZrO_2 | 5m | 81 |
| Zinc manganese oxide (hetaerolite), ZnMn_2O_4 | 10m | 61 | Zirconium phosphide, ZrP | 4m | 75 |
| Zinc molybdenum oxide, $\text{Zn}_2\text{Mo}_3\text{O}_8$ | 7m | 173 | Zirconium silicate, zircon, ZrSiO_4 | 4 | 68 |
| Zinc oxide (zincite), ZnO | 2 | 25 | Zirconium sulfate hydrate, $\text{Zr}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$.. | 7 | 66 |

m—Monograph 25.

A mineral name in () indicates a synthetic sample.

CUMULATIVE ORGANIC INDEX

| | Vol or sec. | Page | | Vol. or sec. | Page |
|--|----------------|------|---|-----------------|------|
| 4-Acetyl-2'-fluorodiphenyl, C ₁₄ H ₁₁ FO | 8m | 91 | 2-Naphthylamine, N-phenyl-, C ₁₀ H ₉ NHC ₆ H ₅ .. | 6m | 29 |
| Alanine, L, CH ₃ CHNH ₂ CO ₂ H | 8m | 93 | Neodymium ethylsulfate hydrate, Nd[(C ₂ H ₅)SO ₄] ₃ ·9H ₂ O | 9 | 41 |
| Ammonium acetate, NH ₄ ·CH ₃ CO ₂ | 8m | 95 | Nickel hexaimidazole nitrate, Ni(C ₃ H ₄ N ₂) ₆ (NO ₃) ₂ | 7m | 27 |
| Ammonium formate, NH ₄ HCO ₂ | 11m | 9 | Nickel tetracyprazole chloride, Ni(C ₃ H ₄ N ₂) ₄ Cl ₂ | 8m | 44 |
| Ammonium oxalate hydrate (oxammite), (NH ₄) ₂ C ₂ O ₄ ·H ₂ O | 7 | 5 | Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazo- cine (alpha HMX) C ₄ H ₈ N ₈ O ₈ | 11m | 100 |
| Ammonium yttrium oxalate hydrate, NH ₄ Y(C ₂ O ₄) ₂ ·H ₂ O | 8m | 97 | Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazo- cine (beta HMX) C ₄ H ₈ N ₈ O ₈ | 11m | 102 |
| Ascorbic Acid, L-C ₆ H ₈ O ₆ | 8m | 99 | Palladium bis-(N-isopropyl-3-ethylsalicy- laldiminate), Pd(C ₁₂ H ₁₆ NO) ₂ | 7m | 144 |
| Azobenzene, C ₆ H ₅ NNC ₆ H ₅ | 7m | 86 | Pimelic acid, (CH ₂) ₅ (CO ₂ H) ₂ | 7m | 153 |
| Cadmium hexaimidazole nitrate, Cd(C ₃ H ₄ N ₂) ₆ (NO ₃) ₂ | 8m | 23 | Potassium formate-formic acid complex, KO ₂ CH·HO ₂ CH | 9m | 93 |
| Calcium formate, Ca(HCO ₂) ₂ | 8 | 16 | Potassium hydrogen o-phthalate, C ₆ H ₄ (COOH)(COOK) | 4m | 30 |
| Calcium malate hydrate, Ca(O ₂ C) ₂ (CH ₂ CHOH)·2H ₂ O | 10m | 76 | Potassium oxalate hydrate, K ₂ C ₂ O ₄ ·H ₂ O | 9m | 39 |
| Copper glutamate hydrate, Cu(O ₂ C) ₂ (H ₂ NCHCH ₂ CH ₂)·2H ₂ O | 7m | 110 | Potassium oxalate perhydrate, K ₂ C ₂ O ₄ ·H ₂ O ₂ | 9m | 96 |
| Copper tetracyprazole chloride, Cu(C ₃ H ₄ N ₂) ₄ Cl ₂ | 8m | 31 | Reserpine, C ₃₃ H ₄₀ N ₂ O ₈ | 8m | 123 |
| Cysteine, L, HSCH ₂ ·CH(NH ₂)·COOH | 11m | 86 | Rubidium oxalate perhydrate, Rb ₂ C ₂ O ₄ ·H ₂ O ₂ | 9m | 102 |
| Dibenzoylmethane, (C ₆ H ₅ CO) ₂ CH ₂ | 7m | 115 | Silver oxalate, Ag ₂ C ₂ O ₄ | 9m | 47 |
| bis-(o-Dodecacarborane), C ₄ B ₂₀ H ₂₂ | 6m | 7 | Sodium D-tartrate hydrate, (CHOH-CO ₂ Na) ₂ ·2H ₂ O | 11m | 110 |
| Glucose, D, alpha, (dextrose), C ₆ H ₁₂ O ₆ | 11m | 28 | Sodium oxalate, Na ₂ C ₂ O ₄ | 6m | 70 |
| Glyoxime, H ₂ C ₂ (NOH) ₂ | 8m | 102 | Strontium formate, Sr(CHO ₂) ₂ | 8 | 55 |
| Hexamethylene diammonium adipate, (CH ₂) ₄ (CO ₂ H ₃ N) ₂ (CH ₂) ₆ | 7m | 121 | Strontium formate hydrate, Sr(CHO ₂) ₂ ·2H ₂ O (orthorhombic) | 8 | 56 |
| Holmium ethylsulfate hydrate, Ho[(C ₂ H ₅)SO ₄] ₃ ·9H ₂ O | 1m | 18 | Sucrose, C ₁₂ H ₂₂ O ₁₁ | 11m | 66 |
| Hydroquinone, gamma, HOC ₆ H ₄ OH | 8m | 107 | Tartaric acid, D, (CHOHCO ₂ H) ₂ | 7m | 168 |
| Iron oxalate hydrate (humboldtine) FeC ₂ O ₄ ·2H ₂ O | 10m | 24 | Trimethylammonium chloride, (CH ₃) ₃ NHCl | 9m | 113 |
| Lead formate, Pb(HCO ₂) ₂ | 8 | 30 | 2,4,6-Trinitrophenetole, C ₂ H ₅ OC ₆ H ₂ (NO ₂) ₃ | 8m | 152 |
| Lithium oxalate, Li ₂ C ₂ O ₄ | 10m | 34 | Urea, CO(NH ₂) ₂ | 7 | 61 |
| Mercury o-phthalate, C ₆ H ₄ (CO ₂ Hg) ₂ | 10m | 113 | Uric acid, C ₅ H ₄ N ₄ O ₃ | 8m | 154 |
| Methyl sulfonanilide, C ₆ H ₅ NHSO ₂ CH ₃ | 9m | 78 | Zinc diimidazole chloride, Zn(C ₃ H ₄ N ₂) ₂ Cl ₂ | 7m | 123 |
| N-Methylphenazinium-7,7,8,8-tetracyanoquinodimethanide, C ₁₄ H ₁₀ N ₆ | 7m | 146 | Zinc glutamate hydrate, Zn(O ₂ CCHNH ₂ CH ₂ CH ₂ CO ₂)·2H ₂ O | 7m | 170 |

CUMULATIVE MINERAL INDEX

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|---|-----------------|------|
| Alabandite, MnS | 4 | 11 | *Diaspore, $\text{Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ | 3 | 41 |
| Alum, $\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$ | 6 | 36 | Diopside, $\text{CaMg}(\text{SiO}_3)_2$ | 5m | 17 |
| Ammonia-niter, NH_4NO_3 | 7 | 4 | *Dravite, $\text{NaMg}_3\text{Al}_6\text{B}_3\text{Si}_6\text{O}_{27}(\text{OH})_4$ | 3m | 47 |
| Anatase, TiO_2 , (revised) | 7m | 82 | Eitelite, $\text{Na}_2\text{Mg}(\text{CO}_3)_2$ | 11m | 56 |
| Andradite, $\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$ | 9 | 22 | Elpasolite, K_2NaAlF_6 | 9m | 43 |
| Anglesite, PbSO_4 | 3 | 67 | *Enstatite, MgSiO_3 | 6 | 32 |
| Anhydrite, CaSO_4 | 4 | 65 | Epsomite, $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ | 7 | 30 |
| Antimony, Sb | 3 | 14 | Eschynite, CeNbTiO_6 | 3m | 24 |
| Aphthitalite, $\text{K}_2\text{Na}(\text{SO}_4)_2$ | 6m | 52 | Eskolaite, Cr_2O_3 | 5 | 22 |
| Aragonite, CaCO_3 | 3 | 53 | Ettringite, $\text{Al}_2\text{O}_3 \cdot 6\text{CaO} \cdot 3\text{SO}_3 \cdot 31\text{H}_2\text{O}$ | 8 | 3 |
| Arcanite, K_2SO_4 | 3 | 62 | Fairchildite, $\text{K}_2\text{Ca}(\text{CO}_3)_2$ | 8m | 48 |
| Argentite, Ag_2S | 10 | 51 | Fluorapatite, $\text{Ca}_5\text{F}(\text{PO}_4)_3$ | 3m | 22 |
| Arsenic, As | 3 | 6 | Fluorite, CaF_2 | 1 | 69 |
| Arsenolite, As_2O_3 | 1 | 51 | Forsterite, Mg_2SiO_4 | 1 | 83 |
| Aurostibite, AuSb_2 | 7 | 18 | Franklinite, ZnFe_2O_4 | 9m | 60 |
| *Azurite, $\text{Cu}_3(\text{OH})_2(\text{CO}_3)_2$ | 10 | 30 | Fresnoite, $\text{Ba}_2\text{TiSi}_2\text{O}_8$ | 9m | 14 |
| Barite, BaSO_4 , (revised) | 10m | 12 | Gahnite, ZnAl_2O_4 | 2 | 38 |
| Berlinite, AlPO_4 | 10 | 3 | Galaxite, MnAl_2O_4 | 9 | 35 |
| Berndtite, SnS_2 | 9m | 57 | Galena, PbS | 2 | 18 |
| *Beryl, $\text{Be}_3\text{Al}_2(\text{SiO}_3)_6$ | 9 | 13 | Geikielite, MgTiO_3 | 5 | 43 |
| Bischofite, $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$ | 11m | 37 | Gersdorffite, NiAsS | 1m | 35 |
| Bismite, (alpha) Bi_2O_3 | 3m | 17 | Glauberite, $\text{Na}_2\text{Ca}(\text{SO}_4)_2$ | 6m | 59 |
| Bismoclite, BiOCl | 4 | 54 | Gold, Au | 1 | 33 |
| Bismuth, Bi | 3 | 20 | Goslarite, $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$ | 8 | 71 |
| Bismuthinite, Bi_2S_3 , (revised) | 5m | 13 | Greenockite, CdS | 4 | 15 |
| *Bloedite, $\text{Na}_2\text{Mg}(\text{SO}_4)_2 \cdot 4\text{H}_2\text{O}$ | 6m | 63 | *Groutite, MnO(OH) | 11m | 97 |
| Böhmite, $\text{Al}_2\text{O}_3 \cdot \text{H}_2\text{O}$ | 3 | 38 | Halite, NaCl | 2 | 41 |
| Bromellite, BeO | 1 | 36 | Hausmannite, Mn_2O_4 | 10m | 38 |
| Bromyrite, AgBr | 4 | 46 | *Hemimorphite, $\text{Zn}_4(\text{OH})_2\text{Si}_2\text{O}_5 \cdot \text{H}_2\text{O}$ | 2 | 62 |
| *Brookite, TiO_2 | 3m | 57 | Hetaerolite, ZnMn_2O_4 | 10m | 61 |
| Brucite, $\text{Mg}(\text{OH})_2$ | 6 | 30 | Hieratite, K_3SiF_6 | 5 | 50 |
| Bunsenite, NiO | 1 | 47 | Huebnerite, MnWO_4 | 2m | 24 |
| Burkeite, $\text{Na}_2\text{CO}_3 (\text{SO}_4)_2$ | 11m | 52 | Humboldtine, $\text{FeC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ | 10m | 24 |
| *Butlerite, $\text{FeSO}_4(\text{OH}) \cdot 2\text{H}_2\text{O}$ | 10m | 95 | Humite, $3\text{Mg}_2\text{SiO}_4 \cdot \text{MgF}_2$ | 1m | 30 |
| Calcite, CaCO_3 | 2 | 51 | Hydrophilite, CaCl_2 | 11m | 18 |
| Calomel, Hg_2Cl_2 | 1 | 72 | Iodyrite, AgI | 8 | 51 |
| Carnallite, $\text{KMgCl}_3 \cdot 6\text{H}_2\text{O}$ | 8m | 50 | Iron, alpha Fe | 4 | 3 |
| Cassiterite, SnO_2 | 1 | 54 | Jacobsite, MnFe_2O_4 | 9 | 36 |
| Celestite, SrSO_4 | 2 | 61 | *Julgoldite, $\text{Ca}_2\text{Fe}_3\text{Si}_3\text{O}_{10}(\text{OH}, \text{O})_2(\text{OH})_2$ | 10m | 72 |
| Cerargyrite, AgCl | 4 | 44 | Langbeinite, $\text{K}_2\text{Mg}_2(\text{SO}_4)_3$ | 6m | 40 |
| Cerianite, CeO_2 | 1 | 56 | Lead, Pb | 1 | 34 |
| Cerussite, PbCO_3 | 2 | 56 | *Leucophanite, $\text{NaCaBeF}_3\text{Si}_2\text{O}_6$ | 8m | 138 |
| Cervantite, Sb_2O_4 | 10 | 8 | Litharge, PbO (red) | 2 | 30 |
| Chalcocyanite, Cu_2S | 3m | 29 | Lithiphosphate, Li_3PO_4 | 4m | 21 |
| Chloraluminite, $\text{AlCl}_3 \cdot 6\text{H}_2\text{O}$ | 7 | 3 | Loellingite, FeAs_2 | 10 | 34 |
| Chlorocalcite, KCaCl_3 | 7m | 36 | Magnesite, MgCO_3 | 7 | 28 |
| Chloromagnesite, MgCl_2 | 11m | 94 | Magnetite, Fe_3O_4 | 5m | 31 |
| Chrysoberyl, BeAl_2O_4 | 9 | 10 | Malachite, $\text{Cu}_2(\text{OH})_2\text{CO}_3$ | 10 | 31 |
| Cinnabar, HgS | 4 | 17 | Manganolangbeinite, $\text{K}_2\text{Mn}_2(\text{SO}_4)_3$ | 6m | 43 |
| *Claudetite, As_2O_3 | 3m | 9 | Manganosite, MnO | 5 | 45 |
| Clausthalite, PbSe | 5 | 38 | Marshite, CuI | 4 | 38 |
| Copper, Cu | 1 | 15 | Mascagnite, $(\text{NH}_4)_2\text{SO}_4$, (revised) | 9 | 8 |
| Cordierite, $\text{Mg}_2\text{Al}_4\text{Si}_5\text{O}_{18}$, (hexagonal) | 1m | 29 | Massicot, PbO (yellow) | 2 | 32 |
| Cordierite, $\text{Mg}_2\text{Al}_4\text{Si}_5\text{O}_{18}$, (orthorhombic) | 1m | 28 | Matlockite, PbFCl_3 | 1 | 76 |
| Corundum, Al_2O_3 | 9 | 3 | Melanterite, $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$ | 8m | 38 |
| Cotunnite, PbCl_2 | 2 | 45 | *Meliphanite, $\text{Na}_{0.63}\text{Ca}_{1.37}\text{BeAl}_{1.13}\text{Si}_{1.87}\text{O}_{6.25}\text{F}_{.75}$ | 8m | 135 |
| Covellite, CuS | 4 | 13 | Metacinnabar, HgS | 4 | 21 |
| Cristobalite, (alpha or low) SiO_2 , (revised) | 10 | 48 | Miargyrite, AgSb_2S_3 | 5m | 49 |
| Cristobalite, (beta or high) SiO_2 | 1 | 42 | *Millerite, NiS | 1m | 37 |
| *Cryolithionite, $\text{Li}_3\text{Na}_3\text{Al}_2\text{F}_{12}$ | 9m | 23 | Minium, Pb_3O_4 | 8 | 32 |
| Cryptohalite, $(\text{NH}_4)_2\text{SiF}_6$ | 5 | 5 | Mitscherlichite, $\text{K}_2\text{CuCl}_4 \cdot 2\text{H}_2\text{O}$ | 9m | 34 |
| Cuprite, Cu_2O | 2 | 23 | Molybdenite, MoS_2 | 5 | 47 |
| *Diamond, C | 2 | 5 | Molybdate, MoO_3 | 3 | 30 |

*Natural mineral.

M—Monograph 25.

CUMULATIVE MINERAL INDEX—Continued

| | Vol. or sec. | Page | | Vol. or sec. | Page |
|---|-----------------|------|---|-----------------|------|
| *Newberryite, $MgHPO_4 \cdot 3H_2O$ | 7m | 139 | *Sodalite, $Na_4Si_6Al_2O_{14}Cl_1$, | 7m | 158 |
| Niter, KNO_3 | 3 | 58 | Soda-niter, $NaNO_3$, | 6 | 50 |
| Nitrobarite, $Ba(NO_3)_2$ (revised) | 11m | 14 | Sphalerite, ZnS | 2 | 16 |
| Norbergite, $Mg_2SiO_4 \cdot MgF_2$ | 10 | 39 | Sphero cobaltite, $CoCO_3$, | 10 | 24 |
| Oldhamite, CaS | 7 | 15 | Spinel, $MgAl_2O_4$ (revised) | 9m | 25 |
| Otavite, $CdCO_3$ | 7 | 11 | Stibnite, Sb_2S_3 | 5 | 6 |
| Oxammite, $(NH_4)_2C_2O_4 \cdot H_2O$ | 7 | 5 | Stolzite, $PbWO_4$ (revised) | 5m | 34 |
| Palladium, Pd | 1 | 21 | Strontianite, $SrCO_3$, | 3 | 56 |
| *Paratellurite, TeO_2 | 10 | 55 | Struvite, $MgNH_4PO_4 \cdot 6H_2O$ | 3m | 41 |
| Paratellurite, TeO_2 | 7 | 56 | Sulfur, S (orthorhombic) | 9 | 54 |
| Partridgeite, alpha Mn_2O_3 (revised) | 11m | 95 | Sylvite, KCl | 1 | 65 |
| Periclase, MgO | 1 | 37 | Tantalum, Ta | 1 | 29 |
| Perovskite, $CaTiO_3$ | 9m | 17 | Tellurium, Te | 1 | 26 |
| *Phenacite, Be_2SiO_4 | 8 | 11 | *Tellurite, TeO_2 | 9 | 57 |
| Picrochromite, $MgCr_2O_4$ | 9 | 34 | Tellurobismuthite, Bi_2Te_3 , | 3m | 16 |
| Picromerite, $K_2Mg(SO_4)_2 \cdot 6H_2O$ | 8m | 54 | Tenorite, CuO | 1 | 49 |
| *Pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$ | 9m | 106 | Teschemacherite, NH_4HCO_3 , | 9 | 5 |
| Platinum, Pt | 1 | 31 | Thenardite, Na_2SO_4 , | 2 | 59 |
| Portlandite, $Ca(OH)_2$ | 1 | 58 | Thermanatrile, $Na_2CO_3 \cdot H_2O$ | 8 | 54 |
| Powellite, $CaMoO_4$ | 6 | 22 | *Thomsenolite, $NaCaAlF_6 \cdot H_2O$ | 8m | 132 |
| Pyrargyrite, Ag_3SbS_3 | 5m | 51 | Thorianite, ThO_2 | 1 | 57 |
| Pyrite, FeS_2 | 5 | 29 | Thortveitite, $Sc_2Si_2O_7$, | 7m | 58 |
| *Pyroaurite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$, phase II | 10m | 104 | Tiemannite, $HgSe$ | 7 | 35 |
| Pyrolusite, $\beta\text{-MnO}_2$ | 10m | 39 | Tin, alpha Sn (cubic) | 2 | 12 |
| Pyrope, $Mg_3Al_2(SiO_4)_3$ | 4m | 24 | Tin, beta Sn (tetragonal) | 1 | 24 |
| *Quartz, SiO_2 (alpha or low) | 3 | 24 | *Topaz, $Al_2SiO_4(F, OH)_2$ | 1m | 4 |
| Rammelsbergite, $NiAs_2$ | 10 | 42 | Trevorite, $NiFe_2O_4$ | 10 | 44 |
| Retgersite, $NiSO_4 \cdot 6H_2O$ | 7 | 36 | Tschermigite, $NH_4Al(SO_4)_2 \cdot 12H_2O$ | 6 | 3 |
| Rhodochrosite, $MnCO_3$ | 7 | 32 | Tungstenite, WS , | 8 | 65 |
| Rutile, TiO_2 , (revised) | 7m | 83 | Uraninite, UO_2 , | 2 | 33 |
| Safflorite, $CoFeAs_4$ | 10 | 28 | Uvarovite, $Ca_2Cr_2(SiO_4)_3$, | 10 | 17 |
| Sal-ammoniac, NH_4Cl | 1 | 59 | *Valentinite, Sb_2O_3 , | 10 | 6 |
| Sanmartinitie, $ZnWO_4$ | 2m | 40 | Villiaumite, NaF | 1 | 63 |
| Scacchite, $MnCl_2$ | 8m | 43 | Willemite, Zn_2SiO_4 , | 7 | 62 |
| *Scheelite, $CaWO_4$ | 6 | 23 | Witherite, $BaCO_3$, | 2 | 54 |
| Selenium, Se | 5 | 54 | Wulfenite, $PbMoO_4$, | 7 | 23 |
| Selenolite, SeO_2 , (revised) | 7m | 60 | Wurtzite, ZnS | 2 | 14 |
| Sellaite, MgF_2 | 4 | 33 | *Xanthoconite, Ag_3AsS_3 , | 8m | 126 |
| Senarmontite, Sb_2O_3 | 3 | 31 | Xenotime, YPO_4 | 8 | 67 |
| Silver, Ag | 1 | 23 | Zinc, Zn | 1 | 16 |
| Silver, Ag (reference standard) | 8m | 2 | Zincite, ZnO | 2 | 25 |
| *Sjögrenite, $Mg_6Fe_2CO_3(OH)_{16} \cdot 4H_2O$, phase I | 10m | 103 | Zinkosite, $ZnSO_4$, | 7 | 64 |
| Skutterudite, $CoAs_3$ | 10 | 21 | *Zircon, $ZrSiO_4$ | 4 | 68 |
| *Smithsonite, $ZnCO_3$ | 8 | 69 | | | |

* U. S. GOVERNMENT PRINTING OFFICE : 1974—542-653/137

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m—Monograph 25.

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|---|--|--|-----------------------------|------------------------------|
| U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET | | 1. PUBLICATION OR REPORT NO. NBS-MN 25, Section 11 | 2. Gov't Accession No. | 3. Recipient's Accession No. |
| 4. TITLE AND SUBTITLE Standard X-ray Diffraction Powder Patterns Section 11 ---- Data for 70 Substances | | 5. Publication Date February 1974 6. Performing Organization Code | | |
| 7. AUTHOR(S) Howard E. Swanson, Howard F. McMurdie, Marlene C. Morris, Elaine H. Evans, Boris Paretzkin, Johan H. de Groot & Simon J. Carmel | | 8. Performing Organization | | |
| 9. PERFORMING ORGANIZATION NAME AND ADDRESS NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20234 | | 10. Project/Task/Work Unit No. 3130163 11. Contract/Grant No. | | |
| 12. Sponsoring Organization Name and Address Same as 9. | | 13. Type of Report & Period Covered Interim 14. Sponsoring Agency Code | | |
| 15. SUPPLEMENTARY NOTES | | | | |
| 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 70 substances. Fifty-two of these patterns represent experimental data and 18 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns. | | | | |
| 17. KEY WORDS (Alphabetical order, separated by semicolons) Crystal structure; integrated intensities; lattice constants; peak intensities, powder patterns; reference intensities; standard; x-ray diffraction | | | | |
| 18. AVAILABILITY STATEMENT <input checked="" type="checkbox"/> UNLIMITED. <input type="checkbox"/> FOR OFFICIAL DISTRIBUTION. DO NOT RELEASE TO NTIS. | | 19. SECURITY CLASS (THIS REPORT) UNCL ASSIFIED | 21. NO. OF PAGES 134 | |
| | | 20. SECURITY CLASS (THIS PAGE) UNCL ASSIFIED | 22. Price \$1.55 | |

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