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Standard X-ray Diffraction Powder Patterns

Section 9—Data for 63 Substances

Howard E. Swanson, Howard F. McMurdie, Marlene C. Morris
Eloise H. Evans, and Boris Paretzkin
Assisted by Johan H. DeGroot and Simon J. Carmel

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CONTENTS

Errata

Monograph 25

Section 8, pg. 12; N_β should be 1.486

Section 8, pgs. 36, 37, 46, 47, 58, 76. Data in the table headings should read: a=3.16516 and λ=1.54056

Section 8, pg. 68; N_α should be 1.6217 and N_β should be 1.6330 and N_γ=1.6435 as given by Tutton

Section 8, pg. 129; both tables are for hexagonal NaN_3 and should appear on page 130.

Section 8, pgs. 130-131; both tables are for monoclinic NaN_3 and should appear on page 129

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

NBS Monograph 25, Sections 1, 2, 3 and NBS Circular 539, Volumes 1 thru 10 may be obtained from Mr. Howard E. Swanson, Room A221, Materials Building, National Bureau of Standards.

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 9 - Data for 63 substances

Howard E. Swanson, Howard F. McMurdie,[1] Marlene C. Morris,[2]
Eloise H. Evans,[2] and Boris Paretzkin[2]
Assisted by Johan H. deGroot[2] and Simon J. Carmel

Standard x-ray diffraction patterns are presented for 63 substances. Forty of these patterns represent experimental data and 23 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 computer 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 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, our 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 63 compounds (40 experimental and 23 calculated patterns), and is the nineteenth 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, recrystallizing, or heating in hydrothermal bombs improved the quality of most of the patterns. A check of phase purity was usually 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, with oils standardized in sodium light, in the refractive index range 1.40 to 2.1. [Hartshorne and Stuart, 1960].

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

Structure, lattice constants. The space groups are 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].

A computer program [Evans et al., 1963] assigned hkℓ's and refined the lattice constants. Cell refinement was based only upon 2θ values which could be indexed without ambiguity. In indexing cubic patterns, multiple hkℓ's were not reported; instead, we chose the single appropriate index having the largest h. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample. Unit cell constants and their standard errors were based on least-squares refinement of the variance-covariance matrix derived from the unweighted $\Delta\theta$ residuals.

Densities. These were calculated from the NBS lattice constants, the Avogadro number (6.06252×10^{23}), and atomic weights based on carbon 12 [International Union, 1961].

Interplanar spacings. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard (approximately 5 wt. percent tungsten powder). When tungsten lines were found to interfere, approximately 25 wt. percent powdered 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 aberrations at the very top of the peak, the reading of 2θ was taken at a position about 20 percent of the way down from the

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

[3] Joint Committee on Powder Diffraction Standards, 1601 Park Lane ,Swarthmore, Pa. 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Society for Testing and Materials, the American Crystallographic Association, The Institute of Physics, the National Association of Corrosion Engineers, the American Ceramic Society, the Mineralogical Society of America, and the Canadian Mineralogical Society.

[4] See previous page for listing of other published volumes.

top, and in the center of the peak width. The internal standard correction appropriate to each region was then applied to the measured value of 2θ. We have reported all data as K_{α_1} peaks because the internal standard corrections for all regions were established in terms of the K_{α_1} wavelength. The lattice constants used for the internal standards at 25 °C are given in the table below. The following angles for high purity (four 9's) tungsten, silver, and cadmium oxide were computed using cell dimensions uncorrected for index of refraction.

All of our spacing determinations were recorded at 25 ± 1 °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 assumed to be 1.54056 Å [Bearden, 1964].

Calculated 2θ Angles

CuK_{α_1} 1.54056Å

hkℓ	W a = 3.16516Å ±.00004	Ag a = 4.08641Å ±.00002	CdO a = 4.69576Å ±.00002
110	40.262		
111		38.112	33.013
200	58.251	44.295	38.304
211	73.184		
220	86.996	64.437	55.287
310	100.632		
311		77.390	65.920
222	114.923	81.533	69.255
321	131.171		
400	153.535	97.875	82.014
331		110.499	91.290
420		114.914	94.378
422		134.871	106.954
511		156.737	116.939
440			136.230
531			152.077
600			159.618

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by [Alexander et al. 1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Fig. 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 Fig. 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 intensity of the strongest line. At least three patterns for intensity measurements were prepared for each sample to check reproducibility.

Reference intensity. For reference intensity measurements, αAl_2O_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 Figs. 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 113 reflection). 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 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 somewhat at NBS.

Lattice parameters. Before the computations of the patterns, corrections were made as necessary in the published parameters to make them consistent with the revised value of the copper wavelength [Bearden, 1964]; specifically, the published parameter in Å was multiplied by 1.00004. Both the altered parameter and the original published value are given.

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] on pages 202 (Table #3.3.1A), 210 (#3.3.1B), 213 (#3.3.2A), and 214 (#3.3.2B). Corrections were made for dispersions if the authors had done so.

Thermal parameters. The computer program uses thermal parameter data of two forms, the isotropic B's and anisotropic β_{ij}'s. The isotropic parameters were used directly, if given by the structure reference. Initially, in a few of our patterns, anisotropic parameters were also used directly as given by the structure reference. In later work, in place of using given anisotropic parameters, we used approximately equivalent isotropic parameters, calculated from the equation:

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

Integrated intensities. Intensity calculations were based on the copper K_{α_1} wavelength, 1.54056 Å, determined by Bearden [1964]. The integrated intensities were computed from formula (1):

$$(1) \qquad I = F^2 \ (Lp) \ (FAC)$$

where F is the standard structure factor

FAC is the powder multiplicity

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

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 had been 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 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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ISCC-NBS Centroid Color Charts, SRM 2106, obtained from the Office of Standard Reference Materials, Room B328, Chemistry Building, National Bureau of Standards, Washington, D.C. 20234. $5.00 per set.

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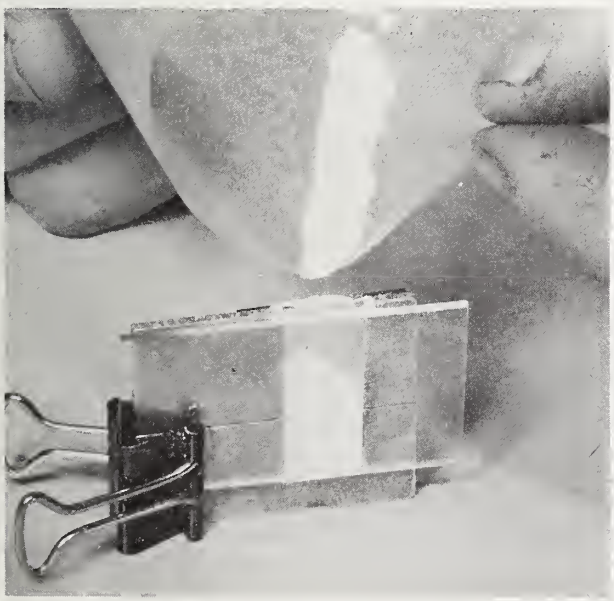

Figure 1

Figure 2

$I/I_{corundum}$ Values for Some Previously Reported Powder Patterns

Aluminum oxide, α–Al_2O_3 (hexagonal)	1.0
Bismuth telluride (tellurobismuthite), Bi_2Te_3 (hexagonal)	6.3
Calcium carbonate, $CaCO_3$ (hexagonal)	2.0
Calcium hydroxide (portlandite), $Ca(OH)_2$ (hexagonal)	1.4
Magnesium, Mg (hexagonal)	2.0
Magnesium hydroxide, $Mg(OH)_2$ (hexagonal)	1.6
Nickel aluminum oxide, $NiAl_2O_4$ (cubic)	1.6
Nickel sulfate hydrate (retgersite) $NiSO_4 \cdot 6H_2O$ (tetragonal)	3.6
Potassium sulfate (arcanite), K_2SO_4 (orthorhombic)	1.8
Rubidium bromide, RbBr (cubic)	7.4
Rubidium chloride, RbCl (cubic)	7.6
Silicon oxide, SiO_2 (hexagonal)	3.6
Silver, Ag (cubic)	5.2
Silver chlorate, $AgClO_3$ (tetragonal)	2.9
Silver iodide, γ–AgI (cubic)	2.6
Silver nitrite, $AgNO_2$ (orthorhombic)	2.5
Silver selenate, Ag_2SeO_4 (orthorhombic)	3.1
Silver sulfate, Ag_2SO_4 (orthorhombic)	2.1
Sodium bromide, NaBr (cubic)	6.8
Sodium iodide, NaI (cubic)	1.2
Tungsten, W (cubic)	18.0
Zinc, Zn (hexagonal)	3.8

Ammonium Aluminum Fluoride, $(NH_4)_3AlF_6$

Sample
The sample was prepared by adding HF to a solution of $AlCl_3$ and NH_4OH, then filtering and washing the precipitate.

Color
Colorless

Optical data
Isotropic, N=1.410

Structure
Cubic, F23 (196) or $F\bar{4}3m$ (216), Z=4, structure determined by Pauling [1924]. Except for hydrogen positions, the structure also satisfies the conditions for Fm3m (225). The compound is isostructural with $(NH_4)_3FeF_6$ and many other hexafluorides.

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.934 ±.001

Density
(calculated) 1.817 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 1.5$

Polymorphism
Steward and Rooksby [1953] found that $(NH_4)_3AlF_6$ has tetragonal or possibly lower symmetry at -180 °C.

Additional patterns
1. PDF card 3-0122 [Dow Chemical Co.] Midland, Mich.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.15	100	111	17.19
4.46	55	200	19.88
3.157	45	220	28.24
2.579	20	222	34.75
2.233	30	400	40.35
2.049	4	331	44.16
1.998	3	420	45.35
1.824	6	422	49.96
1.720	11	511	53.21
1.579	5	440	58.38
1.510	4	531	61.34
1.489	2	600	62.31
1.412	4	620	66.10
1.363	2	533	68.83
1.347	1	622	69.73
1.2900	2	444	73.33
1.2514	2	711	75.98
1.2389	1	640	76.89
1.1941	3	642	80.34
1.1634	1	731	82.92
1.1170	<1	800	87.20
1.0833	1	820	90.64
1.0528	1	822	94.05
1.0314	1	751	96.63
0.9988	<1	840	100.92
.9806	<1	911	103.54
.9524	1	664	107.96
.9366	1	931	110.66
.9118	<1	844	115.29
.8978	1	933	118.17
.8933	1	10·0·0	119.14
.8761	1	10·2·0	123.09
.8637	1	951	126.22
.8597	<1	10·2·2	127.27
.8332	1	953	135.18
.8296	1	10·4·0	136.42
.8155	1	10·4·2	141.65
.8056	2	11·1·1	145.95

References

Pauling, L. (1924). J. Am. Chem. Soc. 46, 2738.
Steward, E.G., and H.P. Rooksby (1953). Acta Cryst. 6, 49.

Ammonium Aluminum Selenate Hydrate, $NH_4Al(SeO_4)_2 \cdot 12H_2O$

Sample
The sample was made by slow evaporation of a 1:1 aqueous solution of $(NH_4)_2SeO_4$ and $Al_2(SeO_4)_3$ at room temperature.

Color
Colorless

Optical data
Isotropic, N=1.486

Structure
Cubic, Pa3 (205), Z=4, $NH_4Al(SeO_4)_2 \cdot 12H_2O$ is isostructural with other α-alums such as $KAl(SO_4)_2 \cdot 12H_2O$ [Haussühl, 1961].

Lattice constants

	a(Å)
NBS, sample at 25 °C	12.4432 ±.0004

Density
(calculated) 1.886 g/cm³ at 25° C.

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

References
Haussühl, S. (1961). Z. Krist. 116, 371.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.17	20	111	12.33
6.22	25	200	14.22
5.56	70	210	15.93
5.08	30	211	17.44
4.41	90	220	20.13
4.15	80	221	21.41
3.75	20	311	23.71
3.59	3	222	24.80
3.452	6	320	25.79
3.327	100	321	26.77
3.110	20	400	28.68
3.017	40	410	29.58
2.931	2	411	30.47
2.856	25	331	31.29
2.783	10	420	32.14
2.714	19	421	32.98
2.655	16	332	33.73
2.540	3	422	35.31
2.487	2	430	36.09
2.440	20	431	36.81
2.311	2	250	38.94
2.272	14	521	39.63
2.199	1	440	41.00
2.167	2	522	41.64
2.105	10	531	42.94
2.074	8	600	43.61
2.046	12	610	44.24
2.019	11	611	44.86
1.967	4	620	46.11
1.943	2	621	46.70
1.919	10	541	47.33
1.898	14	533	47.89
1.877	2	622	48.47
1.856	4	630	49.05
1.835	11	631	49.65
1.760	5	543	51.92
1.743	4	711	52.46
1.725	2	640	53.05
1.710	6	270	53.56
1.693	4	721	54.11

d (Å)	*I*	*hkl*	2θ(°)
1.663	2	642	55.19
1.648	6	722	55.72
1.620	7	731	56.79
1.593	1	650	57.82
1.581	7	732	58.33
1.543	2	810	59.88
1.532	4	811	60.39
1.521	2	733	60.86
1.509	7	820	61.39
1.498	4	821	61.88
1.487	<1	653	62.41
1.4663	3	822	63.38
1.4560	1	830	63.88
1.4459	4	831	64.38
1.4368	3	751	64.84
1.4181	2	832	65.80
1.4092	1	752	66.27
1.3829	6	841	67.70
1.3655	1	911	68.68
1.3498	3	670	69.59
1.3418	2	921	70.07
1.3260	1	664	71.02
1.3186	4	922	71.49
1.3116	3	851	71.93
1.2833	2	932	73.77
1.2571	1	941	75.57
1.2506	2	933	76.04
1.2439	1	10·0·0	76.52
1.2379	4	10·1·0	76.96
1.2204	4	10·2·0	78.27

Ammonium Copper Chloride Hydrate, $(NH_4)_2CuCl_4 \cdot 2H_2O$

Sample
The sample was prepared by slow evaporation at room temperature of a 2:1 aqueous solution of NH_4Cl and $CuCl_2$.

Major impurities
0.001-0.01% each: Al and Mg.

Color
Brilliant greenish blue

Optical data
Uniaxial (-), N_o=1.668, N_e=1.640

Structure
Tetragonal, $P4_2/mnm$ (136), Z=2 [Hendricks and Dickinson, 1927]. The structure was refined by Chrobak [1934]

Lattice constants

	a(Å)	*c*(Å)
NBS, sample at 25 °C	7.594 ±.001	7.967 ±.001

Density
(calculated) 2.005 g/cm³ at 25° C.

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

Additional patterns
1. PDF card 1-211 [Hanawalt et al.,1938]
2. Greenberg and Walden [1940]
3. Chrobak [1934]

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.49	100	101	16.12
5.37	50	110	16.48
3.982	5	002	22.31
3.395	20	210	26.23
3.200	25	112	27.86
3.124	30	211	28.55
2.745	70	202	32.59
2.684	90	220	33.35
2.584	17	212	34.68
2.506	12	103	35.80
2.411	8	301	37.26
2.408	8	310	37.38
2.228	20	222	40.46
2.093	9	213	43.18
2.058	6	312	43.97
2.036	12	321	44.45
1.992	20	004	45.50
1.899	14	400	47.85
1.867	9	114	48.74
1.843	8	410	49.42
1.793	8	411	50.87
1.790	7	330	50.99
1.718	5	214	53.27
1.713	8	402	53.43
1.672	8	412	54.87
1.650	4	323	55.67
1.632	5	332	56.32
1.599	18	224	57.60
1.560	5	105	59.18

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Greenberg, A.L. and G.H. Walden Jr. (1940) Jour. Chem. Phys. 8, 645.
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Hendricks, S.B. and R.G. Dickinson (1927). J. Am. Chem. Soc. 49, 2149.

Ammonium Iron Fluoride, $(NH_4)_3FeF_6$

Sample
The sample was prepared by adding an aqueous solution of $FeCl_3$ to a solution of NH_4F in HF.

Color
Colorless

Optical data
Isotropic, N=1.440

Structure
Cubic, F23 (196) or $F\bar{4}3m$ (216), Z=4, structure determined by Pauling [1924]. Except for the hydrogen positions, the structure also satisfies the conditions for Fm3m (225). The compound is isostructural with $(NH_4)_3AlF_6$ and many other hexafluorides.

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	9.1066 ±.0003

Density
(calculated) 1.970 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 2.1

Polymorphism
Steward and Rooksby [1953] found that $(NH_4)_3FeF_6$ was distorted to a tetragonal cell at -180 °C.

Additional patterns
1. PDF card 5-0223 [Rice et al.,1952]

References

Pauling, L. (1924). J. Am. Chem. Soc. 46, 2738.
Rice, H. M., R. C. Turner and J. E. Brydon (1952). Nature 169, 749.
Steward, E.G.,and H.P. Rooksby (1953).Acta Cryst. 6, 49.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.25	100	111	16.88
4.558	55	200	19.46
3.221	50	220	27.67
2.744	8	311	32.61
2.629	4	222	34.08
2.277	25	400	39.54
2.089	1	331	43.28
2.038	9	420	44.42
1.858	12	422	48.98
1.753	12	511	52.13
1.6099	7	440	57.17
1.5394	8	531	60.05
1.5179	4	600	60.99
1.4399	4	620	64.68
1.3894	2	533	67.34
1.3732	1	622	68.24
1.3144	1	444	71.75
1.2756	2	711	74.29
1.2627	1	640	75.18
1.2168	3	642	78.55
1.1857	1	731	81.03
1.1383	<1	800	85.17
1.1126	<1	733	87.63
1.1044	1	820	88.45
1.0734	1	822	91.71
1.0516	1	751	94.19
1.0448	<1	662	95.00
1.0182	<1	840	98.31
0.9995	1	911	100.82
.9936	<1	842	101.65
.9707	<1	664	105.04
.9548	1	931	107.56
.9292	<1	844	111.98
.9151	1	933	114.65
.9106	<1	10·0·0	115.54
.8931	1	10·2·0	119.19
.8804	1	951	122.06
.8762	1	10·2·2	123.07

Sample

The sample was prepared by heating $CaCO_3$ and $H_2WO_4 \cdot H_2O$ at 700 °C, then adding $BaCO_3$ and heating at 1200 °C for half an hour.

Color

Yellow gray

Structure

Cubic, Fm3m (225), Z=4, isostructural with $(NH_4)_3FeF_6$ [Steward and Rooksby, 1951]. The structure of $(NH_4)_3FeF_6$ was determined by Pauling [1924].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.384 ±.001

Density

(calculated) 6.701 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 8.8$

Additional patterns

1. PDF card 6-400 [Steward and Rooksby, 1951]
2. PDF card 20-210 [Chang et al.,1966]

References

Chang, L.L.Y., M.G.Scroger, and B.Phillips (1966). J. Am. Ceram. Soc. 49, 385.

Pauling, L. (1924). J.Am.Chem.Soc.46,2738.

Steward, E.G.,and H.P. Rooksby (1951).Acta Cryst. 4, 503.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.85	25	111	18.29
4.19	1	200	21.17
2.97	100	220	30.11
2.528	10	311	35.48
2.421	4	222	37.11
2.096	30	400	43.13
1.923	4	331	47.22
1.875	1	420	48.50
1.711	40	422	53.51
1.614	5	511	57.03
1.482	15	440	62.63
1.417	4	531	65.88
1.3256	15	620	71.05
1.2783	2	533	74.11
1.2636	1	622	75.12
1.2100	5	444	79.08
1.1739	2	711	82.02
1.1205	14	642	86.86
1.0915	2	731	89.77
1.0481	2	800	94.60
1.0245	<1	733	97.52
.9882	6	822	102.43
.9682	1	751	105.42
.9373	4	840	110.54
.9204	2	911	113.62
.8939	4	664	119.01
.8789	1	931	122.42
.8557	3	844	128.37
.8426	1	933	132.19
.8222	7	10·2·0	139.06
.8106	1	951	143.72

Barium Chloride, $BaCl_2$, (orthorhombic)

Sample
The sample was obtained from Fisher Scientific Co. Fair Lawn, N. J., and was heated overnight at 875 °C.

Major impurities
0.001-0.01% each: Sr

0.01 -0.1 % each: Ca

Color
Colorless

Optical data
Biaxial, N_α=1.730, N_β=1.736, N_γ=1.741, 2V is very large.

Structure
Orthorhombic, Pnam (62), Z=4, isostructural with $PbCl_2$ [Döll and Klemm, 1939]. The structure was refined by Brackett et al. [1963] and Sahl [1963].

Lattice constants

	a(Å)	b(Å)	c(Å)
NBS, sample at 25 °C - - - -	7.872 ±.001	9.425 ±.001	4.7322 ±.0003

Density
(calculated) 3.939 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.3

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.225	45	011	21.01
4.046	85	120	21.95
3.935	45	200	22.58
3.723	70	111	23.88
3.072	20	121	29.04
3.028	18	201	29.47
3.020		220	29.56
2.916	10	130	30.63
2.879	100	211	31.04
2.617	55	031	34.24
2.546	3	221	35.22
2.529	6	310	35.46
2.482	40	131	36.16
2.456	4	230	36.56
2.366	45	002	38.00
2.355	45	040	38.18
2.292	45	320	39.28
2.231	35	311	40.40
2.178	35	231	41.42
2.042	25	122	44.32
2.037		141	44.44
2.028	25	202	44.64
2.023	25	240	44.77
1.969	10	400	46.07
1.863	4	222	48.85
1.854	8	331	49.11
1.838	4	132	49.55
1.833	4	150	49.71
1.784	6	411	51.15
1.728	3	312	52.96
1.710	13	151	53.56
1.705	8	232	53.72
1.6958	2	421	54.03
1.6696	13	042	54.95
1.6461	30	322	55.80
1.5997	8	251	57.57
1.5732	6	431	58.63
1.5556	3	013	59.36
1.5401	11	160	60.02
1.5364	16	242	60.18
1.5263	5	113	60.62

Polymorphism

$BaCl_2$ is stable in a cubic (fluorite) form above 925 °C. A monoclinic form is mentioned but no stability range defined [Vainshtein, 1948].

Additional patterns

1. PDF card 1-948*[Hanawalt et al.,1938]
2. PDF card 1-1177[Dow Chemical Co.,Midland,Mich.]
3. PDF card 2-794 [Döll and Klemm, 1939]
4. Brackett et al. [1963]
5. Solans-Huguet and Font-Altaba [1968]

* appears to be misnamed "high form"

References

Brackett, E. B., T. E. Brackett, and R. L. Sass (1963). J. Phys. Chem. 67, 2132.

Döll, W. and W. Klemm (1939). Z. anorg. u. allgem. Chem. 241, 239.

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

Sahl, K. (1963). Beitr. Mineral. Petrog. 9, 111.

Solans-Huguet, J. and M. Font-Altaba (1968). Anales Real Soc. Espan. Fis. Quim.Madrid 64, 425.

Vainshtein, B.K. (1948). Dokl. Akad. Nauk. USSR, 60, 1169.

d (Å)	*I*	*hkl*	2*θ*(°)
1.5134	13	402	61.19
1.5107		440	61.31
1.4934	8	412,520	62.10
1.4753	17	511	62.95
1.4648	2	161,203	63.45
1.4593	14	260	63.72
1.4564		351	63.86
1.4469	10	213	64.33
1.4099	6	033	66.23
1.3879	5	133	67.42
1.3495	9	531	69.61
1.3478		360	69.71
1.3383	6	313	70.28
1.3269	6	233,170	70.97
1.3116	3	600	71.93
1.3084	5	062,451	72.13
1.2960	6	361	72.93
1.2913	11	162	73.24
1.2779	4	171	74.14
1.2733	8	442	74.45
1.2637	8	601,620	75.11
1.2617		541	75.25
1.2530	4	611	75.87
1.2417	2	262,333	76.68
1.2302	4	271	77.53
1.2203	1	413	78.28
1.1958	2	153	80.20
1.1830	2	004	81.25
1.1709	9	362,551	82.27
1.1561	2	253	83.56
1.1461	6	640,433	84.46
1.1354	2	124	85.44

Sample

The sample was prepared by heating $BaCl_2 \cdot 2H_2O$ at 70 °C overnight in vacuum. This is the method described by Brackett et al. [1963]. Cubic $BaCl_2$ is stable above 925 °C [Brackett et al. [1963]. It persists at room temperature for several hours however, before reverting to the orthorhombic form.

Major impurities

0.001-0.01% each: Sr

0.01 -0.1 % each: Ca

Color

Colorless

Structure

Cubic, Fm3m (225), Z=4, isostructural with CaF_2 [Vainshtein, 1948].

Lattice constants

	a(Å)
NBS, sample at 25°C	7.311 ±.001

Density

(calculated) 3.539 g/cm³ at 25° C.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	*2θ(°)*
4.23	70	111	20.99
3.66	9	200	24.30
2.586	100	220	34.66
2.205	50	311	40.90
2.110	6	222	42.83
1.8274	16	400	49.86
1.6769	25	331	54.69
1.6348	9	420	56.22
1.4921	40	422	62.16
1.4071	19	511	66.38
1.2924	11	440	73.17
1.2357	16	531	77.12

Additional patterns

1. Solans-Huguet and Font-Altaba [1968*] *intensities based on CaF_2
2. PDF card 1-948 is mislabeled "high-form" but is essentially orthorhombic

Polymorphism

Below 925 °C the stable form of $BaCl_2$ is orthorhombic [Gemsky, 1913].

References

Brackett, E. B., T. E. Brackett and R. L. Sass (1963). J. Phys. Chem. 67, 2132.

Gemsky, H. (1913). Neues Jahr. Mineral. Geol. 36, 513.

Solans-Huguet, J.and M. Font-Altaba(1968). Anales De Quimica 64, 425.

Vainshtein, B.K. (1948). Dokl. Akad. Nauk SSSR 60, 1169.

Barium Titanium Silicate (fresnoite), $Ba_2TiSi_2O_8$

Sample

The sample was prepared at NBS by C. R. Robbins [1970].

Color

Colorless

Optical data

Uniaxial(-) N_o=1.775, N_e=1.765, [Robbins, 1970]

Structure

Tetragonal, P4bm (100), Z=2 [Masse, Grenier and Durif, 1967] and [Moore and Louisnathan, 1967]

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25 °C-----	8.5291 ±.0004	5.2110 ±.0003

Density

(calculated) 4.439 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 4.2

Additional patterns

1. PDF card 11-150* [Rase and Roy, 1955]
2. PDF card 18-197 [Alfors et al., 1965]

* given as $BaTiSiO_5$ however, according to Robbins [1970], 11-150 is the same as fresnoite.

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.03	5	110	14.67
5.22	14	001	16.98
4.267	8	200	20.80
3.947	12	111	22.51
3.816	20	210	23.29
3.301	45	201	26.99
3.077	100	211	28.99
3.017	10	220	29.58
2.697	25	310	33.19
2.607	20	221,002	34.37
2.395	8	311	37.52
2.364	2	320	38.03
2.223	6	202	40.54
2.151	20	212	41.97
2.133	4	400	42.34
2.069	16	410	43.72
2.009	10	330	45.08
1.971	6	222	46.00
1.922	15	411	47.25
1.907	6	420	47.65
1.874	20	312	48.55
1.752	2	322	52.17
1.738	3	003	52.63
1.668	1	113	55.00
1.650	2	402	55.65
1.620	9	412	56.78
1.609	5	203	57.20
1.5913	11	332	57.90
1.5804	11	213	58.34
1.5387	2	422	60.08
1.5154	6	521	61.10
1.5074	5	440	61.46
1.4624	3	530	63.57
1.4218	3	600	65.61
1.4081	3	531,512	66.33
1.4019	2	610	66.66
1.3718	2	601	68.32
1.3536	2	611,522	69.37
1.3305	5	413	70.75
1.3144	3	333	71.75

d (Å)	*I*	*hkl*	2θ(°)
1.3050	4	621,442	72.35
1.3030	4	004	72.48
1.2907	4	541	73.28
1.2754	3	532	74.31
1.2475	3	602	76.26
1.2456	3	204	76.40
1.2327	2	214	77.34
1.2049	2	513	79.48
1.1981	2	622	80.02
1.1959	1	224	80.20
1.1863	2	542	80.98
1.1729	4	314	82.10
1.1703	5	523	82.32
1.1532	1	641	83.82
1.1428	2	721,632	84.76
1.1191	2	533	86.99
1.1117	1	404	87.71
1.1023	2	414	88.66
1.0998	2	603	88.91
1.0934	2	334	89.58
1.0756	1	424	91.47
1.0688	3	651,722	92.22
1.0651	2	623	92.64
1.0570	3	543	93.56
1.0444	1	801	95.04
1.0422	1	005	95.30
1.0368	3	741	95.96
1.0342	2	820	96.28
1.0271	1	115	97.17
1.0125	1	205	99.07
1.0060	2	524	99.93

References

Alfors, J.T., M.C. Stinson, R. A. Mathews, and A. Pabst(1965). Am. Mineralogist 50, 314.

Masse,R., J.C. Grenier,and A. Durif(1967). Bull. Soc. Franc. Mineral.Crist. 90, 20.

Moore,P.B. and J. Louisnathan (1967). Science 156, 1361.

Rase,D.E. and R. Roy (1955). J. Am. Ceram. Soc. 38, 389.

Robbins, C. R. (1970). J. Res. Natl. Bur. Std. A 74A, No. 2, 229.

Sample

The sample was prepared by co-precipitation of the hydroxides by addition of NaOH to a solution of $FeCl_3$ and $CdCl_2$. The product was then washed, heated at 500 °C for three days, ground, and heated for two minutes at 850 °C.

Color

Strong brown

Optical data

Isotropic, N = 2.39 [Roberts and Merwin, 1931]

Structure

Cubic, Fd3M (227), Z = 8, spinel type [Posnjak, 1930].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.6996 ±.0002

Density

(calculated) 5.812 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.9

Additional patterns

1. PDF card 1-1083 [Hanawalt et al., 1938]
2. Posnjak [1930]

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
3.075	60	220	29.01
2.623	100	311	34.15
2.514	8	222	35.69
2.175	5	400	41.48
1.997	3	331	45.38
1.776	20	422	51.41
1.674	35	511	54.78
1.538	35	440	60.12
1.376	7	620	68.10
1.327	9	533	70.96
1.3117	3	622	71.92
1.2182	1	711	78.45
1.1624	8	642	83.01
1.1323	13	731	85.73
1.0874	4	800	90.20
1.0629	1	733	92.89
1.0252	4	822	97.41
1.0044	6	751	100.15
.9980	2	662	101.03
.9550	<1	911	107.53
.9274	1	664	112.31
.9119	4	931	115.28
.8873	7	844	120.36
.8744	1	933	123.51
.8531	6	10·2·0	129.09
.8410	6	951	132.67
.8372	3	10·2·2	133.87

References

Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Posnjak, E. (1930). Am. Jour. Sci. 19, 67.
Roberts, J. and H. E. Merwin (1931). Am. Jour. Sci. 21, 145.

Calcium Titanium Oxide (perovskite), $CaTiO_3$

Sample
The sample was prepared by Coughanour et al. [1955] by mixing equimolar amounts of CaO and TiO_2 and pelletizing at 5000 lb/in^2. The pellets were then heated to 1000 to 1200 °C for four hours in an oxidizing atmosphere.

Color
Yellowish white

Optical data
Almost isotropic, N ≅ 2.4

Structure
Orthorhombic, Pnma (62), Z=4, distorted perovskite [Kay and Bailey, 1957].

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
NBS, sample at 25 °C---------	5.4405 ±.0002	7.6436 ±.0005	5.3812 ±.0003

Density
(calculated) 4.036 g/cm^3 at 25° C.

Reference intensity
$I/I_{corundum}$ = 2.6

Additional patterns.
1. PDF card 8-91 [Murdock, 1951].
2. PDF card 9-365 [Padurow and Schusterius, 1955].
3. Coughanour et al. [1955].

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
3.824	14	101,020	23.24
3.423	3	111	26.01
2.719	40	200	32.92
2.701	100	121,002	33.14
2.563	1	210	34.98
2.428	1	201	37.00
2.413	2	102	37.23
2.313	4	211	38.91
2.303	7	031	39.08
2.217	6	220	40.67
2.201	4	022	40.97
2.121	2	131	42.59
2.050	2	221	44.14
2.040	1	122	44.36
1.911	50	040	47.53
1.860	2	230	48.93
1.856	3	212	49.04
1.757	1	231	51.99
1.752	1	132	52.15
1.746	1	013	52.35
1.719	2	301	53.26
1.710	3	222,141	53.53
1.703	2	103	53.77
1.676	3	311	54.71
1.663	1	113	55.17
1.567	14	321	58.89
1.563	16	240	59.04
1.557	25	042	59.30
1.529	<1	232	60.50
1.4978	<1	142,203	61.90
1.4702	1	051,213	63.19
1.4663	<1	033	63.38
1.4246	1	331	65.46
1.3603	3	400	68.98
1.3522	11	242	69.45
1.3455	5	004	69.85
1.3393	2	410	70.23
1.3190	<1	401	71.46
1.3056	<1	104	72.31
1.2938	1	251	73.08

d (Å)	I	hkl	2θ(°)
1.2913	1	152,233	73.24
1.2780	1	341	74.13
1.2578	<1	313	75.53
1.2356	<1	124	77.13
1.2138	2	402	78.78
1.2088	7	161	79.17
1.1995	1	430	79.91
1.1942	<1	252	80.33
1.1913	<1	214	80.57
1.1622	<1	134	83.02
1.1421	1	351	84.82
1.1399	1	333	85.02
1.1378	1	153	85.22
1.1080	2	440	88.09
1.1000	2	044	88.90
1.0958	1	432	89.33
1.0702	<1	071,314	92.07
1.0668	1	501	92.45
1.0565	1	511	93.62
1.0425	<1	423	95.27
1.0395	<1	324	95.63
1.0274	1	521	97.14
1.0244	3	422	97.51
1.0237	4	361	97.61
1.0202	5	163	98.06
1.0176	6	125	98.39
.9840	1	531	103.04
.9564	2	404	107.30
.9555	1	080	107.44
.9491	<1	414	108.50
.9308	1	541,235	111.69
.9279	<1	424	112.23
.9235	1	531	113.05
.9215	<1	371	113.42
.9066	<1	600	116.34
.9039	1	523	116.89
.9012	4	363,280	117.45
.8997	4	325	117.78

References

Coughanour, L.W., R.S. Roth, S. Marzullo, and F. E. Sennett (1955). J. Res. Natl. Bur. Std. 54, 149.

Kay, H. F. and P. C. Bailey (1957). Acta Cryst. 23, 219.

Murdock, J. (1951). Am. Mineralogist 36, 513.

Padurow, N. N. and C. Schusterius (1955). Ber. Deut. Keram. Ges. 32, 292.

Calcium Tungsten Oxide, Ca_3WO_6

Sample
The sample was prepared by a solid state reaction of $CaCO_3$ and HWO_3 when heated at 1000 °C for 24 hours.

Color
Colorless

Optical data
Low birefringence, N ≅ 2.00

Structure
Monoclinic, $P2_1/n$ (14), Z=2, by analogy of the powder pattern with that of Na_3FeF_6. Steward and Rooksby [1951] considered that the structure of Ca_3WO_6 was similar to $(NH_4)_3FeF_6$ but departed considerably from cubic symmetry, and they suggested that the atomic arrangement might be identical to that of Na_3AlF_6.

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25°C	5.547 ±.001	5.808 ±.001	8.002 ±.001	90.15 ±.01

Density
(calculated) 5.154 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 2.9

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
4.701	60	011	18.86
4.562	45	$\bar{1}$01,101	19.44
4.008	65	110,002	22.16
3.589	4	$\bar{1}$11,111	24.79
2.905	30	020	30.75
2.835	100	$\bar{1}$12	31.53
2.776	30	200	32.22
2.503	2	210	35.85
2.451	16	$\bar{1}$21,121	36.64
2.425	7	013	37.04
2.403	16	$\bar{1}$03	37.39
2.393	20	$\bar{2}$11	37.56
2.350	4	022	38.26
2.283	2	$\bar{2}$02	39.43
2.278	4	202	39.53
2.220	4	113	40.60
2.164	3	$\bar{1}$22,122	41.71
2.005	30	220	45.18
2.002	30	004	45.26
1.964	2	023	46.19
1.945	3	$\bar{2}$21,221	46.65
1.882	4	031	48.32
1.853	8	$\bar{1}$23	49.13
1.827	12	130,$\bar{2}$13	49.87
1.802	6	$\bar{3}$01,301	50.62
1.791	17	222,$\bar{1}$14	50.94
1.762	4	310	51.84
1.721	2	$\bar{3}$11,311	53.19
1.662	18	$\bar{1}$32,132	55.21
1.648	14	024	55.75
1.624	8	$\bar{2}$04	56.62
1.620	13	204	56.78
1.614	20	$\bar{3}$12	57.02
1.611	19	312	57.11
1.566	2	033	58.91
1.558	8	$\bar{2}$31,231	59.28
1.543	4	015	59.90
1.538	4	$\bar{1}$05	60.11
1.531	4	$\bar{3}$21	60.40
1.522	3	$\bar{3}$03	60.82

d (Å)	*I*	*hkl*	2*θ*(°)
1.518	2	303	61.00
1.507	2	133	61.47
1.452	3	322,040	64.09
1.417	8	$\bar{2}24$	65.85
1.415	10	224	65.96
1.386	6	400	67.51
1.384	6	$\bar{1}41$,141	67.63
1.365	6	$\bar{2}33$,042	68.71
1.360	6	$\bar{1}25$	68.97
1.349	8	410,134	69.65
1.337	2	330	70.35
1.331	4	$\bar{4}11$	70.74
1.324	2	$\bar{3}14$	71.13
1.321	2	314	71.36
1.312	2	$\bar{4}02$	71.90
1.309	2	402	72.10
1.266	10	$\bar{1}16$	74.93

Additional patterns

1. PDF card 20-244 [Chang et al., 1966].
2. Baglio, J.A. and S. Natansohn [1969].

References

Chang, L.L.Y., M.G. Scroger, and B. Phillips (1966). J. Am. Ceram. Soc. 49, 385.

Steward, E. G. and H. P. Rooksby (1951). Acta Cryst. 4, 503.

Baglio, J.A. and S. Natansohn (1969). J. Appl. Cryst. 2, 252.

Cobalt Chromium Oxide, $CoCr_2O_4$

Sample

The sample was made by heating a mixture of CoO and Cr_2O_3 overnight at 900 °C., grinding, and reheating for 17 hours at 1200 °C.

Color

Dark bluish green

Structure

Cubic, Fd3m (227), Z=8, spinel type [Natta and Passerini, 1929].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.3299 ±.0002

Density

(calculated) 5.215 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 1.8$

Additional patterns

1. PDF card 1-1122 [New Jersey Zinc Co., Palmerton, Pa.]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.82	14	111	18.41
2.947	35	220	30.30
2.512	100	311	35.72
2.405	8	222	37.36
2.084	25	400	43.39
1.700	12	422	53.90
1.6027	35	511	57.45
1.4721	45	440	63.10
1.4081	2	531	66.33
1.3171	4	620	71.58
1.2702	10	533	74.66
1.2556	5	622	75.68
1.2023	3	444	79.68
1.1664	1	711	82.65
1.1131	5	642	87.58
1.0844	14	731	90.52
1.0409	4	800	95.46
.9818	2	822	103.36
.9618	7	751	106.42
.9554	4	662	107.46
.9313	4	840	111.61
.9141	1	911	114.84
.8880	2	664	120.33
.8732	7	931	123.81
.8502	13	844	129.92
.8168	3	10·2·0	141.12
.8053	10	951	146.08

References

Natta, G., and L. Passerini (1929). Gazz. Chim. Ital. 59, 280.

Sample

The sample was prepared by adding $Co(OH)_2$ dissolved in NaOH to a $FeCl_3$ solution acidified with HCl. This mixture was heated to 80 °C while $CoFe_2O_4$ was precipitated by adding NaOH to a pH of 10. The precipitate was heated to 950 °C in air for 40 hours.

Color

Black

Structure

Cubic, Fd3m (227), Z=8, spinel type [Natta and Passerini, 1929].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.3919 ±.0001

Density

(calculated) 5.304 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.7$

Additional patterns

1. PDF card 1-1121, incorrectly labelled $CoFe_3O_4$ [New Jersey Zinc Co., Palmerton, Pa.]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.847	10	111	18.29
2.968	30	220	30.08
2.531	100	311	35.44
2.424	8	222	37.06
2.099	20	400	43.06
1.926	1	331	47.16
1.713	10	422	53.45
1.615	30	711	56.97
1.483	40	440	62.57
1.419	3	531	65.75
1.3273	4	620	70.95
1.2798	9	533	74.01
1.2652	4	622	75.01
1.2114	2	444	78.97
1.1749	2	551	81.93
1.1214	4	642	86.77
1.0925	2	731	89.67
1.0490	5	800	94.50
.9891	2	822	102.30
.9690	8	751	105.29
.9627	4	662	106.29
.9382	4	840	110.38
.9213	1	911	113.46
.8946	2	664	118.87
.8797	6	931	122.24
.8564	14	844	128.16
.8434	1	933	131.93
.8229	3	10·2·0	138.80
.8112	8	951	143.43
.8075	2	10·2·2	145.07

References

Natta, G., and L. Passerini (1929). Gazz. Chim. Ital. 59, 280.

Lithium Sodium Aluminum Fluoride, cryolithionite, $Li_3Na_3Al_2F_{12}$

Sample

A natural mineral from Ivigtut, Greenland (National Museum #94311) was used. It contained a few percent of Na_3AlF_6 and these lines were disregarded. An analysis by Menzer [1930] of material from this locality indicated that the cryolithionite had total impurities of less than 0.3 weight percent, and that the Na to Li ratio was 3:2.82.

Major impurities

0.001-0.01% each: Ag, Ba, Ca, Cu, Ni, Pb, Si, and Ti.
0.01 -0.1 % each: Cr and Fe.

Color

Colorless

Optical data

Isotropic, N=1.340

Structure

Cubic, Ia3d (230), Z=8, garnet type. The structure was determined by Menzer[1930] and refined by Geller [1971].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	12.1254 ±.0002

Density

(calculated) 2.770 g/cm³ at 25° C. (based on a Na to Li ratio of 1:1).

Reference intensity

$I/I_{corundum} = 1.0$

Additional patterns

1. PDF card 2-1282 [Menzer, 1930]

References

Geller, S. (1971). Am. Mineralogist 56, 18.
Menzer, G. (1930). Z. Krist. 75, 265.

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.95	13	211	17.89
4.28	100	220	20.73
3.243	5	321	27.48
3.029	55	400	29.46
2.711	35	420	33.02
2.584	17	332	34.68
2.477	1	422	36.24
2.376	35	431	37.83
2.213	50	521	40.74
2.144	6	440	42.11
1.966	55	611	46.13
1.917	20	620	47.39
1.788	2	631	51.05
1.750	10	444	52.24
1.715	5	543	53.38
1.681	16	640	54.53
1.649	11	721	55.69
1.619	30	642	56.81
1.539	7	732	60.05
1.515	9	800	61.12
1.493	3	811	62.15
1.470	2	820	63.20
1.449	2	653	64.21
1.429	8	822	65.24
1.410	3	831	66.25
1.373	2	752	68.26
1.356	12	840	69.25
1.324	2	842	71.18
1.3077	2	921	72.18
1.2928	6	664	73.14
1.2780	4	851	74.13
1.2509	2	932	76.02
1.2378	3	844	76.97
1.2252	8	941	77.91
1.2011	1	10·1·1	79.78
1.1895	2	10·2·0	80.72
1.1564	2	10·3·1	83.53
1.1261	3	10·4·0	86.32
1.1163	3	10·3·3	87.26
1.1072	5	10·4·2	88.17

d (Å)	*I*	*hkl*	2θ(°)
1.0980	2	873	89.10
1.0804	2	11·2·1	90.95
1.0716	2	880	91.91
1.0475	2	11·3·2	94.67
1.0400	1	10·6·0	95.58
1.0248	1	10·6·2	97.46
1.0177	2	965	98.38
1.0107	2	12·0·0	99.30
1.0035	<1	12·1·1	100.27
.9965	<1	12·2·0	101.24
.9903	<1	11·5·2	102.13
.9836	3	12·2·2	103.09
.9772	1	12·3·1	104.04
.9646	1	11·6·1	105.98
.9413	2	11·6·3	109.84
.9356	<1	10·8·2	110.83
.9193	1	13·2·1	113.83
.9139	<1	12·4·4	114.89
.9037	3	12·6·0	116.94
.8987	1	13·3·2	117.98
.8939	2	12·6·2	119.02
.8890	1	13·4·1	120.10
.8750	1	888	123.37
.8705	1	13·4·3	124.48
.8617	1	14·1·1	126.74
.8573	2	14·2·0	127.93
.8448	1	14·3·1	131.51
.8408	1	12·8·0	132.74
.8328	1	14·4·0	135.33
.8249	7	14·4·2	138.05
.8212	3	12·7·5	139.43
.8138	1	14·5·1	142.36

Sample

The sample was furnished by H. R. Shell of the Bureau of Mines, College Park,Md. He used a carbon electrode furnace and removed an excess of MgO with hot HCl after crushing.

Color

Colorless

Optical data

Isotropic, N=1.718

Structure

Cubic, Fd3m (227), Z=8. The structure was determined by Bragg [1915] and Nishikawa [1915]. Atomic parameters were refined by Bacon [1952], using neutron defraction.

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.0831 ±.0001

Density

(calculated) 3.578 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.7

Additional patterns

1. PDF card 5-672[Swanson and Fuyat,1953]

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.66	35	111	19.02
2.858	40	220	31.27
2.437	100	311	36.84
2.335	3	222	38.53
2.020	65	400	44.83
1.650	9	422	55.64
1.5554	45	511	59.37
1.4289	55	440	65.24
1.3662	3	531	68.64
1.2780	3	620	74.13
1.2330	8	533	77.32
1.2187	1	622	78.40
1.1666	5	444	82.64
1.1320	2	711	85.76
1.0802	5	642	90.97
1.0524	12	731	94.10
1.0104	7	800	99.34
0.9527	2	822	107.90
.9334	8	751	111.22
.9274	1	662	112.32
.9038	6	840	116.91
.8872	1	911	120.50
.8820	<1	842	121.69
.8616	<1	664	126.76
.8474	8	931	130.74
.8249	17	844	138.07
.8123	<1	933	142.97
.7927	2	10·2·0	152.70
.7814	11	951	160.65

References

Bacon, G.E. (1952). Acta Cryst. **5**, 684.
Bragg, W.H. (1915). Nature **95**, 561.
Nishikawa, S. (1915). Proc. Math. Phys. Soc., Tokyo, 8, 199.
Swanson, H.E.,and R.K. Fuyat (1953). Natl. Bur. Std. U.S. Circ. 539, II, 35.

Magnesium Sulfite Hydrate, $MgSO_3 \cdot 6H_2O$

Sample
The sample was formed by precipitation when aqueous solutions of $MgCl_2 \cdot 6H_2O$ and H_2SO_3 were mixed.

Color
Colorless

Optical data
Uniaxial (-), N_o=1.51, N_e=1.46

Structure
Hexagonal, R3 (146), Z=3. The structure was determined by Klasens et al. [1935].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25 °C	8.8385 ±.0004	9.080 ±.001

Density
(calculated) 1.723 g/cm³ at 25° C.

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

Major impurities
0.001-0.01% each: Ca and Fe

0.01 -0.1 % each: Na

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.85	12	101	15.14
4.416	85	110	20.09
3.905	100	012	22.75
3.524	4	021	25.25
3.025	65	003	29.50
2.926	30	202	30.53
2.758	50	211	32.43
2.552	4	300	35.14
2.497	10	113	35.94
2.439	30	122	36.82
2.208	2	220	40.83
2.178	4	104	41.43
2.067	7	131	43.75
1.952	10	024,303	46.49
1.924	12	312	47.21
1.872	2	401	48.60
1.786	30	214,223	51.11
1.767	1	015	51.70
1.764	1	042	51.77
1.725	2	321	53.05
1.670	13	410	54.93
1.638	3	232	56.09
1.551	3	134	59.56
1.538	2	125	60.10
1.513	<1	006	61.19
1.510	1	051	61.33
1.473	<1	330	63.08
1.463	3	404,413	63.56
1.451	1	502	64.11
1.4315	3	116	65.11
1.3892	4	324	67.35
1.3784	3	422	67.95
1.3591	<1	511	69.05
1.3160	2	152	71.65
1.3014	2	306	72.58
1.2789	3	107	74.07
1.2756	2	600	74.29
1.2484	2	226	76.20
1.2466	3	431	76.33
1.2254	5	520	77.89

d (Å)	*I*	*hkl*	2*θ*(°)
1.2198	2	244	78.32
1.2125	2	342	78.88
1.1839	<1	217	81.18
1.1759	<1	514,603	81.85
1.1701	<1	505	82.34
1.1363	<1	523	85.36
1.1311	1	425	85.84
1.1216	2	416	86.75
1.1070	<1	137	88.19
1.1045	1	440	88.43
1.1007	1	434	88.82
1.0883	<1	208	90.11
1.0856	<1	351	90.40
1.0632	1	072	92.85
1.0566	<1	128	93.60
1.0554	<1	336	93.74
1.0434	<1	327	95.16
1.0380	<1	164,443	95.82
1.0333	1	262	96.40
1.0138	<1	710	98.89

Additional patterns

1. PDF card 1-0473 [Hanawalt et al., 1938]

References

Klasens, H.A.,W.G. Perdok, and P. Terpstra (1935). Rec. Trav. Chim. 44, 728.

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

Manganese Chloride Hydrate, $MnCl_2 \cdot 4H_2O$

Sample
The sample was recrystallized from an aqueous solution at room temperature.

Color
Light pink

Optical data
Biaxial(+), N_α=1.583, N_β=1.608, N_γ=1.667
2V is large.

Structure
Monoclinic, $P2_1/n$ (14), Z=4. The structure was determined by Zalkin et al. [1964].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	11.194 ±.001	9.527 ±.002	6.202 ±.001	99.75 ±.01

Density
(calculated) 2.016 g/cm³ at 25° C.

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

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.23	4	110	12.24
5.52	40	200	16.04
5.15	8	011	17.22
5.00	13	$10\bar{1}$	17.74
4.943	100	$\bar{1}11$	17.93
4.766	25	210,020	18.60
4.429	75	111	20.03
4.371	25	$12\bar{0}$	20.30
4.064	20	$\bar{2}11$	21.85
3.760	6	021	23.64
3.675	6	$\bar{1}21$	24.20
3.600	5	220	24.71
3.519	11	211	25.29
3.450	5	121	25.80
3.433	7	310	25.93
3.268	18	$\bar{2}21$	27.27
3.218	11	$\bar{3}11$	27.70
3.057	40	002	29.19
2.913	75	320,012	30.67
2.817	15	031	31.74
2.808	12	311	31.84
2.778	25	$\bar{3}21$	32.19
2.762	35	$\bar{2}12$	32.39
2.753	40	230	32.50
2.709	30	112	33.04
2.595	45	$\bar{2}31$	34.54
2.589	20	$\bar{4}11,\bar{1}22$	34.62
2.572	7	022	34.86
2.499	17	321,202	35.90
2.485	20	$\bar{3}12$	36.12
2.435	10	231	36.89
2.403	9	330	37.40
2.387	9	420	37.66
2.343	12	$\bar{4}21$	38.38
2.328	8	140,$\bar{3}31$	38.65
2.299	4	411	39.15
2.265	7	$\bar{3}22$	39.77
2.212	9	222,$\bar{1}32$	40.75
2.198	15	$\bar{5}01$	41.03
2.185	6	240,$\bar{4}12$	41.29

d (Å)	*I*	*hkl*	2*θ*(°)
2.149	13	141,510	42.01
2.142	19	$\bar{5}11$	42.16
2.121	5	312,421	42.60
2.054	20	$\bar{4}31$	44.06
2.031	10	$\bar{4}22$	44.57
2.018	10	$\bar{2}41$	44.89
1.999	18	$\bar{3}32$,340	45.34
1.979	25	322	45.81
1.946	3	103	46.63
1.931	6	511	47.01
1.905	17	113	47.70
1.898	19	431	47.89
1.886	20	$\bar{1}42$	48.21
1.871	8	023	48.62
1.858	5	412	48.99
1.839	6	600,$\bar{2}42$	49.52
1.833	5	$\bar{4}32$	49.69
1.817	6	$\bar{6}11$	50.16
1.809	17	$\bar{1}51$	50.40
1.806	8	$\bar{5}22$,610	50.50
1.780	9	151	51.29

Additional patterns

1. PDF card 1-0362 [Hanawalt et al., 1938]

References

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

Zalkin, A., J. D. Forrester and D. H. Templeton (1964). Inorg. Chem. 3, 529.

Sample

$MnCl_2$ and $CoCl_2$ in a molar ratio of 1:2 were treated with HNO_3. The product was dried, heated to 760 °C for one hour and then heated overnight at 720 °C.

Color

Opaque black

Structure

Cubic, Fd3m (227), Z=8, spinel type [Holgersson and Karlsson, 1929].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.269 ±.001

Density

(calculated) 5.564 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.3

Additional patterns

1. PDF card 1-1130[Hanawalt et al., 1938]

Internal standard Ag, a = 4.08641 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.78	14	111	18.54
2.925	35	220	30.54
2.493	100	311	36.00
2.388	10	222	37.64
2.067	20	400	43.76
1.687	9	422	54.33
1.5911	30	511	57.91
1.4613	35	440	63.62
1.3976	2	531	66.89
1.3077	3	620	72.18
1.2610	6	533	75.30
1.2463	5	622	76.35
1.1935	2	444	80.39
1.1579	1	711	83.40
1.1047	3	642	88.42
1.0764	9	731	91.38
1.0336	3	800	96.35
0.9746	2	822	104.44
.9550	5	751	107.52

References

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

Holgersson, S., and A. Karlsson (1929). Z. anorg. u. allgem. Chem. 183, 384.

Potassium Aluminum Sulfate, $KAl(SO_4)_2$

Sample
The sample was prepared by heating $KAl(SO_4)_2 \cdot 12H_2O$ at 700 °C for 15 hours.

Color
Colorless

Optical data
Uniaxial (-), N_o=1.546, N_e=1.533

Structure
Hexagonal, P321 (150), Z=1, isostructural with many other dehydrated alums. The structure was determined by Vegard and Maurstad [1929].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25°C	4.7194 ±.0001	7.9833 ±.0003

Density
(calculated) 2.784 g/cm³ at 25° C.

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

Additional patterns
1. PDF card 3-337, Dow Chemical Co.,Midland, Michigan

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
7.986	25	001	11.07
4.088	4	100	21.72
3.638	100	101	24.45
2.858	50	102	31.27
2.663	15	003	33.63
2.361	25	110	38.08
2.264	8	111	39.78
2.032	4	112	44.56
1.996	1	004	45.40
1.980	4	201	45.78
1.819	13	202	50.10
1.794	9	104	50.86
1.766	<1	113	51.72
1.621	2	203	56.74
1.597	<1	005	57.66
1.5448	1	210	59.82
1.5238	6	114	60.73
1.5170	7	211	61.03
1.4872	2	105	62.39
1.4405	8	212	64.65
1.4279	4	204	65.29
1.3625	8	300	68.85
1.3358	1	213	70.43
1.3309	1	006	70.73
1.3224	3	115	71.25
1.2652	2	106	75.01
1.2580	1	205	75.51
1.2215	3	214	78.19
1.2127	2	303	78.87
1.1798	2	220	81.52
1.1591	1	116	83.30
1.1222	3	311	86.69
1.1150	2	206	87.39
1.1106	1	215	87.83
1.0985	<1	107	89.05
1.0904	3	312	89.89
1.0787	<1	223	91.14
1.0363	1	305	96.03
1.0267	1	117	97.22
1.0156	1	224	98.65
1.0134	1	401	98.95
1.0081	2	216	99.65
.9898	2	402	102.19
.9858	2	314	102.78
.9694	<1	108	105.24
.9518	<1	306	108.06
.9489	1	225	108.53
.9312	1	321	111.62
.9190	<1	118	113.89
.9129	2	322	115.09
.8967	<1	208	118.42
.8918	2	410	119.48
.8629	2	316	126.42

References
Vegard, L. and A. Maurstad (1929). Z. Krist. 69, 519.

Sample

The sample was prepared from an aqueous solution of $BaCl_2$, $NiCl_2$ and KNO_2 according to the method given by Ferrari and Colla [1931].

Color

Medium yellow

Optical data

Isotropic, N=1.598

Structure

Cubic, Fm3m (225), Z=4, isostructural with other hexanitrites [Ferrari and Colla, 1933]; structure of this group of compounds was determined by van Driel and Verweel [1936].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	10.797 ±.001

Density

(calculated) 2.904 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.9$

Additional patterns

1. Ferrari and Colla [1931]

References

van Driel, M., and H.J. Verweel (1936). Z. Krist. 95, 308.

Ferrari, A., and C. Colla (1931), Atti reale accad. nazl. Lincei 14, 435.

Ferrari, A., and C. Colla (1933). Atti reale accad. nazl. Lincei 17, 390.

Internal standard W, a = 3.16516 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.22	15	111	14.22
5.39	90	200	16.43
3.815	100	220	23.30
3.254	30	311	27.39
2.699	95	400	33.17
2.477	25	331	36.24
2.414	55	420	37.22
2.203	85	422	40.93
2.078	9	511	43.51
1.9080	20	440	47.62
1.8247	7	531	49.94
1.7994	11	600	50.69
1.7069	20	620	53.65
1.6464	5	533	55.79
1.6277	6	622	56.49
1.5580	3	444	59.26
1.5114	3	711	61.28
1.4969	7	640	61.94
1.4423	25	642	64.56
1.4056	6	731	66.46
1.3492	5	800	69.63
1.3187	3	733	71.48
1.3094	5	820	72.07
1.2721	8	822	74.53
1.2470	3	751	76.30
1.2387	5	662	76.90
1.2072	6	840	79.30
1.1851	3	911	81.08
1.1782	4	842	81.65
1.1507	3	664	84.04
1.1316	1	931	85.80
1.1018	3	844	88.71
1.0852	2	933	90.43
1.0796	3	10·0·0	91.03
1.0586	6	10·2·0	93.38
1.0439	3	951	95.10
1.0390	3	10·2·2	95.69
1.0069	3	953	99.82
1.0025	5	10·4·0	100.42
.9858	6	10·4·2	102.78
.9735	1	11·1·1	104.60
.9542	2	880	107.65
.9433	3	971	109.48
.9398	4	10·4·4	110.09
.9260	3	10·6·0	112.59

Potassium Calcium Nickel Nitrite, $K_2CaNi(NO_2)_6$

Sample

The sample was prepared from an aqueous solution of $CaCl_2$, $NiCl_2$ and KNO_2 according to the method given by Ferrari and Colla [1931].

Color

Medium yellow

Optical data

Isotropic, N=1.640

Structure

Cubic, Fm3m (225), Z=4, structure determined by van Driel and Verweel [1936], isostructural with other hexanitrites [Ferrari and Colla, 1933].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	10.361 ±.001

Density

(calculated) 2.705 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.6

Additional patterns

1. PDF card 3-837,(Michigan Alkali Co. Wyandotte, Michigan)
2. van Driel and Verweel [1936]
3. Ferrari and Colla [1931]

Internal standard W, a = 3.16516 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.98	6	111	14.80
5.18	40	200	17.12
3.66	55	220	24.27
3.124	3	311	28.55
2.993	30	222	29.83
2.591	100	400	34.59
2.377	2	331	37.81
2.317	45	420	38.84
2.116	75	422	42.69
1.994	5	511	45.44
1.833	18	440	49.71
1.752	3	531	52.17
1.726	2	600	53.01
1.638	15	620	56.09
1.495	2	444	62.02
1.450	3	711	64.17
1.4366	3	640	64.85
1.3847	25	642	67.60
1.3488	2	731	69.65
1.2950	5	800	73.00
1.2659	2	733	74.96
1.2207	4	822	78.25
1.1964	2	751	80.16
1.1886	3	662	80.79
1.1584	5	840	83.36
1.1310	2	842	85.85
1.1045	6	664	88.44
1.0576	3	844	93.49
1.0161	5	10·2·0	98.59

References

van Driel, M., and H.J. Verweel (1936), Z. Krist. 95, 308.

Ferrari, A., and C. Colla (1931), Atti reale accad. nazl. Lincei 14, 435.

Ferrari, A., and C. Colla (1933), Atti reale accad. nazl. Lincei 17, 390.

Potassium Copper Chloride Hydrate (mitscherlichite), $K_2CuCl_4 \cdot 2H_2O$

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

Color
Brilliant greenish blue

Optical data
Uniaxial (-), N_o=1.638, N_e=1.613

Structure
Tetragonal $P4_2/mnm$ (136), Z=2, isostructural with $(NH_4)_2CuCl_4 \cdot 2H_2O$ and $Rb_2CuCl_4 \cdot 2H_2O$ [Hendricks and Dickinson, 1927]. The structure was refined by Chrobak [1934].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25°C	7.454 ±.001	7.909 ±.001

Density
(calculated) 2.416 g/cm³ at 25° C.

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

Additional patterns
1. Chrobak [1934]
2. PDF card 1-1073 [Hanawalt et al.,1938]
3. PDF card 13-203 [Kleber and Steinike-Hartung, 1959]

Major impurities
0.01 -0.1 % each: Si

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.42	70	101	16.34
5.27	7	110	16.81
3.96	20	002	22.44
3.73	6	200	23.82
3.335	14	210	26.71
3.164	50	112	28.18
3.072	25	211	29.04
2.711	95	202	33.01
2.635	100	220	34.00
2.549	12	212	35.18
2.486	11	103	36.10
2.371	5	301	37.91
2.192	7	222	41.15
2.067	9	213,320	43.76
2.024	14	312	44.75
1.999	9	321	45.33
1.977	25	004	45.86
1.864	17	223,400	48.82
1.807	5	303,410	50.46
1.763	3	411	51.82
1.701	2	214	53.87
1.643	5	412	55.88
1.627	4	323	56.51
1.606	5	332	57.31
1.5814	25	224	58.30
1.5476	3	105	59.70

References

Chrobak, L. (1934). Z. Krist. 88, 35.
Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem. Anal.Ed.10, 457.
Hendricks, S.B. and R.G. Dickinson (1927). J. Am. Chem. Soc. 49, 2149.
Kleber, W. and U. Steinike-Hartung (1957). Z. Krist. 111, 213.

Potassium Iron Cyanide, $K_3Fe(CN)_6$

Sample
The sample was obtained from City Chemical Corp., New York, N.Y.

Color
Deep reddish orange

Optical data
Biaxial(+) N_α=1.561, N_β=1.562, N_γ=1.576, 2V is medium.

Structure
Monoclinic, $P2_1/c$ (14), Z = 4 [Gottfried and Nagelschmidt, 1930].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25°C	13.471 ±.002	10.417 ±.001	8.402 ±.001	90.11 ±.01

Density
(calculated) 1.855 g/cm³ at 25° C.

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

Polymorphism
$K_3Fe(CN)_6$ is reported to undergo a change in crystalline state at about 130 °K [Barros and Oosterhuis, 1970].

Additional patterns
1. PDF card 1-423 [Hanawalt et al.,1938]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
6.74	12	200	13.12
6.54	3	011	13.53
5.90	2	$\bar{1}11$,111	15.00
5.21	7	020	16.99
4.691	2	$\bar{2}11$,211	18.90
4.120	100	310,220	21.55
4.012	20	$\bar{1}02$,102	22.14
3.742	3	$\bar{1}12$,112	23.76
3.367	7	212,400,+	26.45
3.205	5	031,410	27.81
3.178	4	$\bar{1}22$,122	28.05
3.086	30	230	28.91
3.067	35	302	29.09
2.945	45	$\bar{3}12$,$\bar{2}22$	30.32
2.938		312,222	30.40
2.641	25	322	33.91
2.625	20	402,132	34.14
2.605	15	040	34.40
2.448	1	$\bar{1}41$,141	36.68
2.429	2	240,$\bar{1}23$	36.97
2.300	4	521,$\bar{3}32$,+	39.14
2.265	4	502	39.76
2.215	7	512,042	40.70
2.183	9	142	41.32
2.097	10	$\bar{4}32$,432	43.10
2.077	14	522,$\bar{1}04$,+	43.54
2.059	25	440,014	43.93
1.986	2	$\bar{3}42$,342	45.65
1.938	<1	$\bar{2}51$,251	46.84
1.899	1	$\bar{5}32$	47.85
1.885	1	630	48.25
1.870	7	224,314	48.65
1.828	1	433,$\bar{5}41$,+	49.83
1.781	3	134,404	51.26
1.772	<1	450	51.54
1.756	1	$\bar{3}43$,414	52.05
1.748	1	702	52.28
1.735	1	060,234	52.70
1.7230	3	352,160	53.11
1.7099	1	542	53.55

d (Å)	I	hkl	2θ(°)
1.6812	6	260	54.54
1.6571	2	722	55.40
1.6341	2	514,$\bar{4}$52	56.25
1.6027	1	820	57.45
1.5926	3	$\bar{1}$62,162	57.85
1.5616	<1	802,732	59.11
1.5429	1	460	59.90
1.5341	1	$\bar{5}$52,552	60.28
1.5107	1	$\bar{3}$62,362	61.31
1.5025	<1	135,$\bar{6}$51,+	61.68
1.4893	<1	$\bar{4}$15	62.29
1.4694	8	624,444,+	63.23
1.4514	2	742	64.11
1.4133	1	$\bar{5}$15,750	66.05
1.4287	1	902	66.25
1.3961	1	544,912	66.97
1.3919	1	$\bar{8}$23	67.20
1.3790	1	$\bar{5}$62,435	67.91
1.3750	1	930	68.14
1.3725	1	272	68.28
1.3597	1	$\bar{2}$16,922	69.01

References

Barros, F.de S. and W.T. Oosterhuis(1970). J. Phys. Chem. 3, 279.

Gottfried, C. and J.G. Nagelschmidt(1930). Z. Krist. 73, 357.

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

Potassium Iron Fluoride, K_3FeF_6

Sample

The sample was prepared by adding a solution of $FeCl_3$ in HF to a solution of KF with an excess of HF.

Color

Colorless

Optical data

Isotropic, N ≅ 1.410, (sample was very fine grained)

Structure

Cubic, Fm3m (225), Z=4, [Bode and Voss, 1957]. Peacock [1957] found K_3FeF_6 to be tetragonal with a=8.59 and c=8.66. Our sample showed no evidence of being non-cubic.

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.622 ±.001

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.98	30	111	17.79
4.312	17	200	20.58
3.048	100	220	29.28
2.598	3	311	34.50
2.490	8	222	36.04
2.155	40	400	41.88
1.978	3	331	45.84
1.929	3	420	47.08
1.760	25	422	51.92
1.658	7	511	55.35
1.524	11	440	60.74
1.457	4	531	63.82
1.437	3	600	64.84
1.364	5	620	68.78
1.3151	1	533	71.71
1.2446	3	444	76.47
1.2074	3	711	79.28
1.1519	4	642	83.93

Density

(calculated) 2.975 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.4$

Additional patterns

1. PDF card 3-0589 [Dow Chemical Co.] Midland, Mich.

References

Bode, H., and E. Voss (1957). Z. Anorg. Allgem. Chem. 290, 1.

Peacock, R. D. (1957). J. Chem. Soc. 1957, 4684.

Sample
Reagent grade KNO_2 was obtained from Allied Chemical Co., Morristown, N.J. The sample was maintained in a dry atmosphere.

Color
Colorless

Optical data
Uniaxial (-) N_o=1.466, N_e<1.400

Structure
Hexagonal, $R\bar{3}m$ (166), Z=3 [Chang, 1963], [Tanisaki and Ishimatsu, 1965]. KNO_2 was earlier reported to be monoclinic [Ziegler, 1936].

Lattice constants

	a(Å)	*c*(Å)
NBS, sample at 25 °C-----	4.994 ±.001	10.253 ±.001

Density
(calculated) 1.914 g/cm³ at 25° C.

Polymorphism
KNO_2 undergoes a phase transition at 70°C, above which it is cubic [Tanisaki and Ishimatsu, 1965].

Additional patterns
1. PDF card 1-668 [Hanawalt et al.,1938]
2. Ziegler [1936]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
3.98	4	101	22.31
3.42	<1	003	26.07
3.304	100	012	26.96
2.497	12	110	35.94
2.205	25	104	40.89
2.117	5	021	42.67
2.016	6	113	44.92
1.992	4	202	45.49
1.855	2	015	49.08
1.709	2	006	53.58
1.653	1	024	55.54
1.615	2	211	56.96
1.557	<1	122	59.29
1.488	<1	205	62.35
1.441	<1	300	64.61
1.410	1	116	66.23
1.387	<1	107	67.48
1.378	1	214	67.95
1.328	1	303	70.89
1.279	<1	125	74.07
1.229	<1	018	77.61
1.213	<1	027	78.86

References
Chang, Sh-C. (1963). Dissertation Abstr. **24**, 1668.
Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem., Anal. Ed. **10**, 457.
Tanisaki, S., and T. Ishimatsu (1965). J. Phys. Soc. Japan, **20**, 1277.
Ziegler, G. E. (1936). Z. Krist. **94**, 491.

Potassium Oxalate Hydrate, $K_2C_2O_4 \cdot H_2O$

Sample

The sample was reagent grade material recrystallized from aqueous solution.

Color

Colorless

Optical data

Biaxial(+) N_α=1.440, N_β=1.496, N_γ=1.562. 2V is very large.

Structure

Monoclinic, A2/a (15), Z=4 [Hendricks, 1935]. Two refinements of the structure have been published [Chidambaram et al., 1964] and [Pedersen, 1964].

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	10.684 ±.001	6.182 ±.001	9.226 ±.001	110.77 ±.01

Density

(calculated) 2.148 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 1.0

Additional patterns

1. PDF card 14-760[Hanawalt et al.,1938]

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.024	20	011	17.64
4.990	25	200	17.76
4.916	30	$\bar{1}11$	18.03
4.316	20	002	20.56
4.160	5	111	21.34
4.048	25	$\bar{2}02$	21.94
3.980	4	$\bar{2}11$	22.32
3.225	10	211	27.64
3.087	40	020,$\bar{3}11$	28.90
2.954	35	120	30.23
2.807	100	202	31.85
2.749	25	$\bar{1}13$	32.54
2.695	14	$\bar{2}13$	33.21
2.628	5	220	34.09
2.606	35	013	34.38
2.598		$\bar{4}02$	34.49
2.563	25	$\bar{1}22$	34.98
2.546	10	311	35.22
2.497	55	400	35.93
2.456	75	$\bar{2}22$	36.56
2.447	60	$\bar{4}11$	36.69
2.327	8	122	38.66
2.266	15	320	39.75
2.240	5	$\bar{3}22$	40.23
2.188	6	$\bar{4}13$	41.22
2.156	12	004	41.86
2.079	14	222	43.50
2.026	20	$\bar{4}04$	44.69
2.004	10	031,$\bar{5}11$	45.20
1.943	6	420	46.72
1.916	3	$\bar{2}31$	47.42
1.910	8	$\bar{5}13$	47.58
1.891	2	402	48.08
1.845	2	$\bar{2}24$	49.35
1.835	4	$\bar{1}24$	49.64
1.833	9	322	49.71
1.809	10	231	50.40
1.793	5	$\bar{3}24$,313	50.90
1.780	5	$\bar{6}02$	51.27
1.769	8	024,$\bar{2}15$	51.61
1.750	1	$\bar{5}22$	52.23

d (Å)	*I*	*hkl*	2θ(°)
1.744	3	$\bar{3}15$	52.43
1.738	6	$\bar{1}15,511$	52.61
1.697	4	$\bar{2}33$	53.98
1.687	1	$\bar{6}11$	54.32
1.677	2	520	54.68
1.664	4	600	55.14
1.660	5	124	55.29
1.631	2	$\bar{4}31$	56.38
1.6125	3	422	57.07
1.5706	5	$\bar{5}24$	58.74
1.5686	3	$413,\bar{5}15$	58.82
1.5554	2	115	59.37
1.5429	4	$\bar{6}22$	59.90
1.5332	6	$\bar{2}06,224$	60.32
1.4971	2	$233,\bar{4}06$	61.93
1.4910	1	611	62.21
1.4644	4	$\bar{1}42$	63.47
1.4538	5	$\bar{7}11$	63.99
1.4435	2	$\bar{2}42$	64.50
1.4266	1	522	65.36
1.4160	2	142	65.91
1.4043	5	404	66.53
1.3961	3	$\bar{3}42,602$	66.97
1.3861	2	333,513	67.52
1.3745	5	$\bar{2}35$	68.17
1.3507	2	$\bar{6}06$	69.54
1.3364	2	$\bar{6}31$	70.39
1.3320	1	$\bar{8}02$	70.66
1.3274	2	$\bar{4}42,\bar{4}35$	70.94
1.3253	4	$\bar{6}33$	71.07
1.2991	3	$\bar{5}26,\bar{8}04$	72.73
1.2789	3	424,342	74.07
1.2749	3	$\bar{8}11,433$	74.34
1.2489	2	$\bar{5}42,800$	76.16
1.2374	2	$\bar{6}26$	77.00

References

Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem.Anal.Ed. **10**, 457.
Hendricks, S.B. (1935). Z. Krist. **91**, 48.
Chidambaram, R.,A. Sequeira, and S.K. Sikka (1964). J. Chem. Phys. **41**, 3616.
Pedersen, B.F. (1964). Acta Chem. Scand. **18**, 1635.

Potassium Selenate, K_2SeO_4

Sample

The sample was precipitated by adding H_2SeO_4 to K_2CO_3 in solution.

Color

Colorless

Optical data

Biaxial(+) N_α=1.535, N_β=1.539, N_γ=1.545, 2V is large [Tutton, 1897].

Structure

Orthorhombic, Pnam (62), Z=4 [Gattow, 1962], isostructural with βK_2SO_4. The structure was refined by Kálmán et al. [1970].

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
NBS, sample 25 °C	7.654 ±.001	10.468 ±.001	5.996 ±.001

Density

(calculated) 3.058 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum}$ = 2.0

Additional patterns

1. PDF card 1-857 [Hanawalt et al., 1938]

Internal standard W, a = 3.16516 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
5.23	17	020	16.94
4.320	80	120	20.54
4.304		111	20.62
3.827	30	200	23.22
3.594	5	210	24.75
3.506	<5	121	25.38
3.226	12	201	27.63
3.175	5	130	28.08
3.091	70	220	28.86
3.083		211	28.94
3.015	100	031,002	29.60
2.803	<5	131	31.90
2.747	7	221	32.57
2.695	<5	112	33.22
2.617	17	040	34.23
2.602		022	34.44
2.579	11	230	34.76
2.477	7	310,140	36.24
2.370	8	231	37.94
2.362	5	202	38.07
2.301	30	212	39.11
2.289		311,141,+	39.33
2.180	7	132	41.39
2.160	30	240	41.78
2.151		222	41.96
2.060	<5	330	43.92
2.032	<5	241	44.55
2.019	<5	150	44.85
1.976	<5	051	45.88
1.955	9	232	46.40
1.914	11	151,400	47.47
1.910	11	312,142	47.57
1.902	6	113	47.78
1.837	5	250	49.58
1.827	7	340	49.87
1.821	5	322	50.05
1.772	<5	203	51.53
1.744	9	060	52.42
1.735	11	033	52.73
1.676	6	152	54.73

d (Å)	I	hkl	2θ(°)
1.636	<5	161	56.16
1.616	9	431	56.95
1.594	6	412	57.80
1.587	5	260	58.07
1.580	<5	233	58.34
1.5657	<5	252	58.94
1.5623	7	351	59.08
1.5600	6	342	59.18
1.5561	5	313,143	59.34
1.5345	<5	261	60.26
1.5076	9	062,323	61.45
1.4991	7	004	61.84
1.4673	10	170,243	63.33
1.4638	7	432	63.50
1.4505	<5	071	64.15
1.4459	<5	053	64.38
1.4340	<5	333	64.98
1.4258	<5	171	65.40
1.4166	<5	124	65.88
1.4132	<5	450	66.06
1.4024	9	262,530	66.63
1.3960	<5	204	66.98
1.3927	<5	270	67.16
1.3823	<5	403	67.73
1.3566	<5	271	69.19
1.3551	<5	134	69.28
1.3519	5	253,512	69.47
1.3483	5	224,343	69.68
1.3188	<5	172	71.47
1.3081	<5	080	72.15
1.3006	<5	044	72.63
1.2897	<5	180,460+	73.35

References

Gattow, G. (1962). Acta Cryst., 15, 419.
Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem. Anal.Ed.10, 457.
Kálmán, A., J. S. Stephens, and D. W. J. Cruickshank (1970). Acta Cryst., B26, 1451.
Tutton, A.E.H. (1897). J. Chem. Soc., 71, 846.

Potassium Sodium Aluminum Fluoride (elpasolite), K_2NaAlF_6

Sample
Made by dissolving aluminum in HF, adding K_2CO_3 and Na_2CO_3, drying, melting, and annealing 72 hours at 650 °C.

Color
Colorless

Optical data
Isotropic, N=1.376 [Frondel,1948].

Structure
Cubic, Fm3m (225), Z=4, by analogy with K_3FeF_6 and other hexafluorides. Helmholz [1959] also obtained data consistent with Fm3m using a synthetic sample of K_2NaAlF_6 in which a small amount of aluminum was replaced by iron. The natural mineral elpasolite, K_2NaAlF_6, has been reported to have space group Pa3 (205) [Frondel, 1948],[Menzer, 1932]. Steward and Rooksby [1953] gave the space group Pa3 (205) but their photographed pattern as published does not show the extra lines that would require Pa3.

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.1220 ±.0001

Density
(calculated) 3.002 g/cm³ at 25° C.

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

Additional patterns
1. PDF card 8-70 [Frondel, 1948]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.687	20	111	18.92
4.059	4	200	21.88
2.868	100	220	31.16
2.345	75	222	38.35
2.030	90	400	44.59
1.864	4	331	48.82
1.817	1	420	50.18
1.658	30	422	55.35
1.5633	6	333	59.04
1.4356	35	440	64.90
1.3730	1	531	68.25
1.3539	1	600	69.35
1.2841	12	620	73.72
1.2245	7	622	77.96
1.1722	8	444	82.16
1.1373	2	711	85.27
1.0854	11	642	90.42
1.0572	2	731	93.54
1.0152	3	800	98.71
0.9924	<1	733	101.83
.9851	<1	820	102.88
.9572	4	822	107.16
.9378	<1	751	110.45
.9318	1	662	111.52
.9081	7	840	116.04
.8915	<1	911	119.55
.8862	<1	842	120.74
.8659	4	664	125.64
.8513	1	931	129.59
.8289	6	844	136.63
.8162	1	933	141.32
.7964	8	10·2·0	150.57

References

Frondel, C.(1948). Am.Mineralogist 33, 84.
Helmholz, L. (1959). J.Chem.Phys. 31, 172.
Menzer, G. (1932). Fortschr.Mineral.Krist. Petrog. 17, 439.
Steward, E. G., and H. P. Rooksby (1953). Acta Cryst. 6, 49.

Sample
The sample was precipitated by adding a solution of Rb_2CO_3 to one of H_2SeO_4.

Major impurities
0.01 -0.1 % each: Al, Ba, Cr, and Na

0.1 -1.0 % each: Mg

Color
Colorless

Optical data
Biaxial(+), N_α=1.535, N_β=1.539, N_γ=1.545, 2V is large [Tutton, 1897].

Structure
Orthorhombic, Pnam (62), Z=4, isostructural with K, Cs, and Tl selenates and with β-K_2SO_4 [Gattow, 1962]. The structure of K_2SeO_4 was determined by Kálmán et al. [1970].

Lattice constants

	a(Å)	b(Å)	c(Å)
NBS, sample at 25 °C --------	7.979 ±.001	10.820 ±.001	6.174 ±.001

Density
(calculated) 3.919 g/cm³ at 25° C.

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

References
Gattow, G. (1962). Acta Cryst. 15, 419.
Kálmán, A., J. S. Stephens, and D. W. J. Cruickshank (1970). Acta Cryst. B26, 1451.
Tutton, A.E.H. (1897). J. Chem. Soc. 71, 846.

Internal standard Ag, a = 4.08641 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.42	4	020	16.35
4.48	7	120	19.81
4.451	9	111	19.93
3.990	16	200	22.26
3.740	11	210	23.77
3.626	18	121	24.53
3.351	14	201	26.58
3.285	11	130	27.12
3.212	100	220	27.74
3.202		211	27.84
3.113	92	031	28.66
3.088	60	002	28.89
2.902	2	131	30.76
2.849	9	221	31.37
2.704	13	040	33.10
2.676	16	230	33.46
2.584	25	310	34.69
2.543	4	122	35.27
2.454	4	231	36.59
2.383	20	311,212	37.72
2.366	13	141	37.99
2.251	8	132	40.03
2.239	14	240	40.25
2.225	30	321,222	40.50
2.142	8	330	42.15
2.105	5	241	42.93
2.088	10	150	43.29
2.042	2	051	44.32
2.023	10	331,232	44.77
1.994	10	400	45.46
1.982	6	312	45.75
1.962	1	410	46.23
1.901	4	250	47.80
1.898	10	401	47.88
1.870	7	123,411	48.65
1.829	3	203	49.81
1.813	16	341,242	50.29
1.802	20	060,213	50.57
1.787	17	033	51.08
1.759	2	332,160	51.94
1.745	9	430,133	52.38

d (Å)	*I*	*hkl*	2θ(°)
1.730	7	152	52.88
1.692	4	161	54.16
1.680	7	431,350	54.59
1.675	8	402	54.74
1.656	2	412	55.45
1.643	4	260	55.90
1.631	1	233	56.38
1.619	2	351,252	56.82
1.617	2	342	56.91
1.611	1	313	57.13
1.605	2	143	57.38
1.587	4	261	58.06
1.558	9	062	59.27
1.543	7	004	59.87
1.530	8	520	60.44
1.520	6	432	60.91
1.500	2	071	61.81
1.491	1	053	62.20
1.487	1	521	62.42
1.4671	1	450	63.34
1.4503	12	361,262	64.16
1.4324	2	403	65.06
1.4204	1	531,413	65.68
1.3961	4	253	66.97
1.3938	5	343	67.10
1.3912	5	224	67.24
1.3745	8	540	68.17
1.3709	4	522	68.37
1.3618	2	172	68.89
1.3529	1	080	69.40
1.3414	1	541	70.09
1.3370	5	234	70.36
1.3307	4	433	70.74
1.3070	3	461	72.22
1.3036	5	181	72.44
1.2913	2	620	73.24
1.2842	2	550,263	73.71
1.2705	2	244	74.64
1.2656	1	443	74.98
1.2572	3	551	75.57
1.2527	3	513	75.89
1.2389	2	082	76.89

Sample
The sample was obtained from the reaction of solutions of KCN and $AgNO_3$.

Major impurities
0.001-0.01% each: Al, Ca, Cr, Fe, Si.

0.01 -0.1 % each: Ba and Mg.

Color
Colorless

Optical data
Uniaxial (+), N_o=1.685, N_e=1.93 [Winchell and Winchell, 1964].

Structure
Hexagonal, R3m (160), Z=3. Structure proposed by Braekken [1929].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25 °C	6.0047 ±.0004	5.2570 ±.0005

Density
(calculated) 4.063 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 4.0

Polymorphism
A cubic form of AgCN, with AgBr in solid solution, is reported by Natta and Vecchia [1933].

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
3.699	45	101	24.04
3.001	100	110	29.75
2.345	18	012	38.35
2.329		021	38.62
1.848	9	202	49.26
1.841		211	49.48
1.7528	4	003	52.14
1.7333	8	300	52.77
1.5745	3	122	58.58
1.5132	4	113	61.20
1.5008	4	220	61.76
1.3908	2	131	67.26
1.2740	2	104	74.40
1.2645	2	312	75.06
1.2620	1	401	75.23
1.2321	2	303	77.39
1.1730	2	024	82.09
1.1636	2	321	82.90
1.1403	1	223	84.99
1.1349	1	410	85.49

Additional patterns
1. PDF card 1-859 [Hanawalt et al.,1938]

References
Braekken, H. (1929). Kgl. Norske Vidensk. Selskabs Forh. II 1929, 123.

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

Natta, G., and O. Vecchia (1933). Gazz. Chim. Ital. 63, 439.

Winchell, A.N. and H. Winchell (1964)."The Microscopic Characters of Artificial Inorganic Solid Substances" Academic Press New York and London.

Silver Oxalate, $Ag_2C_2O_4$

Sample
The sample was obtained from the City Chemical Corp., New York, N.Y.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z=2. It was assumed to be isostructural with $Na_2C_2O_4$ [Jeffrey and Parry, 1954].

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	9.368 ±.001	6.2039 ±.0003	3.4556 ±.0003	97.63° ±.01

Density
(calculated) 5.065 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum} = 3.2$

Additional patterns
1. PDF card 14-777 [Griffith, 1943]

References
Griffith, R.L.(1943).J.Chem.Phys. 11, 499.
Jeffrey, G.A., and G.S. Parry (1954). J. Am. Chem. Soc. 76, 5283.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.16	55	110	17.17
4.65	12	200	19.08
3.363	13	$\bar{1}01$	26.48
3.102	35	020	28.76
2.996	100	011	29.80
2.957	4	$\bar{1}11$	30.20
2.760	85	111	32.41
2.664	5	$\bar{2}11$	33.61
2.579	10	220	34.75
2.464	20	$\bar{3}01$	36.43
2.395	8	211	37.52
2.322	20	400	38.75
2.300	6	021	39.14
2.280	25	$\bar{1}21$	39.49
2.187	10	121	41.25
2.158	17	301	41.83
2.018	19	130	44.88
1.949	14	$\bar{4}11$	46.57
1.930	25	$\bar{3}21$	47.05
1.889	1	230	48.13
1.859	5	420	48.97
1.771	30	321,031	51.57
1.740	5	411	52.54
1.719	18	330	53.23
1.713	14	002	53.43
1.6932	2	$\bar{2}31$	54.12
1.6623	6	$\bar{1}12$	55.21
1.6177	5	231	56.87
1.5906	2	112	57.93
1.5507	8	040	59.57
1.5473	10	600	59.71
1.5410	10	202,$\bar{3}12$	59.98
1.4991	7	022	61.84
1.4749	2	$\bar{4}02$	62.97
1.4709	3	240	63.16
1.4566	4	$\bar{4}31$	63.85
1.4533	3	122	64.01
1.4449	9	$\bar{6}11$	64.43
1.4086	3	$\bar{1}41$	66.30
1.3847	13	312,620	67.60
1.3634	2	431	68.80
1.3318	3	$\bar{4}22$,241	70.67
1.3248	3	$\bar{1}32$	71.10
1.3144	7	611	71.75
1.3124	6	$\bar{3}41$	71.88
1.2971	4	710	72.86
1.2897	4	440	73.35
1.2600	4	341	75.37
1.2326	2	$\bar{6}02$	77.35
1.2298	2	150	77.56
1.2066	3	$\bar{6}31$	79.34
1.1960	3	$\bar{7}21$	80.19
1.1851	1	701	81.08
1.1709	2	332	82.27
1.1666	4	051	82.64
1.1513	4	350,151	83.99
1.1494	4	042	84.16

Sample
The sample was prepared by heating $Na_2CrO_4 \cdot 4H_2O$ at 600 °C for 60 hours.

Color
Brilliant yellow

Optical data
Biaxial (+), N_α= 1.765, N_γ= 1.788, 2V is large.

Structure
Orthorhombic, Amam (63), Z=4. The structure was determined by Miller [1936]; the space group designation was corrected by Niggli [1954].

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
NBS, sample at 25 °C	7.1462 ±.0004	9.2635 ±.0004	5.8640 ±.0003

Density
(calculated) 2.771 g/cm³ at 25° C.

Reference intensity
$I/I_{corundum}$ = 1.2

Additional patterns
1. PDF card 1-927 [Hanawalt et al.,1938]

References
Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938).Ind. Eng. Chem. Anal.Ed. 10, 845.
Miller, J.J. (1936). Z. Krist. 94, 131.
Niggli, A. (1954). Acta Cryst. 7, 776.

Internal standard W, a = 3.16516 Å
$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.96	20	011	17.88
4.64	4	020	19.12
4.073	65	111	21.80
3.885	65	120	22.87
3.574	40	200	24.89
2.932	60	002	30.46
2.897	100	211	30.84
2.733	70	031	32.74
2.553	5	131	35.12
2.477	25	022	36.23
2.342	4	122	38.41
2.317	3	040	38.83
2.203	3	140	40.93
2.171	13	231	41.56
2.119	8	320	42.63
2.036	19	222	44.46
1.944	12	240	46.68
1.848	4	113	49.27
1.795	15	331	50.81
1.787	18	400	51.08
1.761	3	142	51.87
1.715	4	151	53.38
1.686	8	213	54.37
1.681	6	411	54.55
1.661	6	340	55.27
1.651	11	033	55.63
1.6195	19	242	56.80
1.6089	1	133	57.21
1.5836	2	251	58.21
1.5438	2	060	59.86
1.5256	4	402	60.65
1.5090	3	160	61.39
1.4951	14	431	62.02
1.4661	7	004	63.39
1.4493	2	422	64.21
1.4453	1	342	64.41
1.4187	5	351	65.77
1.3718	5	124	68.32
1.3664	4	062,520	68.63
1.3570	4	333	69.17

d (Å)	I	hkl	2θ(°)
1.3419	5	162	70.06
1.3215	2	153	71.31
1.3014	4	224	72.58
1.2762	2	262	74.25
1.2737	2	442	74.42
1.2587	1	253	75.46
1.2385	1	044,522	76.92
1.2132	7	433	78.83
1.2058	1	324	79.41
1.1912	1	600	80.58
1.1850	2	362	81.09
1.1705	5	244	82.31
1.1682	2	460	82.50
1.1577	2	611,080	83.42
1.1485	1	115	84.24
1.1451	3	513	84.55
1.1432	2	180	84.72
1.1332	3	404	85.65
1.1112	1	551	87.77
1.1062	2	215	88.27
1.0963	1	035	89.28
1.0917	1	631	89.75
1.0849	2	462	90.47
1.0838	1	135	90.58
1.0769	1	082	91.33
1.0732	2	622	91.74
1.0650	2	182	92.65
1.0632	1	064	92.85
1.0478	2	273	94.64
1.0417	1	380	95.37
1.0189	1	264	98.23
1.0136	1	091	98.92
1.0110	1	613	99.27
1.0035	2	191	100.28
0.9962	2	642,335	101.29

Sodium Chromium Oxide Hydrate, $Na_2CrO_4 \cdot 4H_2O$

Sample

The sample was obtained from J.T. Baker Chemical Co., Phillipsburg, N.J. and was recrystallized from aqueous solution at room temperature.

Color

Brilliant yellow

Optical data

Biaxial(+) N_α=1.564, N_β=1.568, N_γ=1.590, 2V≅5°.

Structure

Monoclinic, $P2_1/c$ (14), [Geslin et al., 1968]. Z is assumed to be 4.

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	6.199 ±.001	11.183 ±.001	12.218 ±.001	104.94 ±.01

Density

(calculated) 1.899 g/cm³ at 25° C.

Additional patterns

1. PDF card 1-334 [Hanawalt et al.,1938]
2. Geslin et al. [1968].

References

Geslin, M., M. Gaultier and G. Pannetier (1968). Bull.Soc.Chim.France, 1968#3,939

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

Internal standard Ag, a = 4.08641 Å

CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
8.12	6	011	10.89
5.99	11	100	14.78
5.91	20	002	14.97
5.60	8	020	15.82
5.29	45	$\bar{1}11$,110	16.74
5.224	7	012	16.96
5.055	80	021	17.53
4.878	5	$\bar{1}02$	18.17
4.467	100	$\bar{1}12$	19.86
4.088	13	$\bar{1}21$,120	21.72
3.712	10	013	23.95
3.666	12	$\bar{1}21$	24.26
3.569	30	$\bar{1}13$	24.93
3.555	40	031,112	25.03
3.216	55	023	27.72
3.170	45	$\bar{1}31$	28.13
3.162		130	28.20
3.122	10	$\bar{1}23$	28.57
3.113	6	122	28.65
2.995	25	200	29.81
2.989		$\bar{2}11$	29.87
2.963	50	$\bar{1}32$	30.14
2.895	20	$\bar{2}12$,210	30.86
2.865	20	$\bar{1}14$	31.19
2.855	25	014	31.31
2.795	3	040	32.00
2.719	14	041	32.91
2.712	16	$\bar{2}21$	33.00
2.658	17	211	33.68
2.647	11	$\bar{1}33$	33.83
2.641	8	132,220,+	33.92
2.614	5	123	34.27
2.535	11	$\bar{1}41$,140	35.38
2.529	9	042	35.47
2.468	4	$\bar{2}23$	36.38
2.458	4	221	36.52
2.426	8	$\bar{1}42$,141	37.02
2.412	8	104	37.24
2.383	3	$\bar{2}14$,$\bar{2}31$	37.72
2.359	4	114	38.12

d (Å)	I	hkl	2θ(°)
2.339	4	$\bar{2}32$	38.46
2.315	9	133,034	38.87
2.278	5	043	39.52
2.245	20	$\bar{1}43$	40.14
2.222	5	$\bar{1}25$	40.56
2.212	3	$\bar{2}33$	40.75
2.197	2	051	41.05
2.176	4	025	41.47
2.103	4	$\bar{2}15$	42.97
2.095	14	150,213,+	43.15
2.041	3	$\bar{2}34$	44.34
2.036	4	232,$\bar{1}$44	44.45
2.031	11	143,$\bar{1}$06,+	44.58
2.029		044,$\bar{1}$35	44.62
2.026	12	134,$\bar{3}$12	44.70
2.022	3	$\bar{3}11$	44.79
1.994	4	035,115	45.45
1.967	4	006	46.10
1.960	5	$\bar{2}43$	46.29
1.939	7	016	46.81
1.931	14	$\bar{3}22$,$\bar{3}21$	47.02
1.923	15	$\bar{1}53$	47.23
1.904	4	125	47.73
1.897	5	$\bar{3}04$	47.92
1.875	7	204	48.52
1.864	10	060,311	48.82
1.856	7	026,$\bar{2}$16,+	49.03
1.838	9	$\bar{2}44$	49.56
1.803	11	045,$\bar{3}$32	50.58
1.784	10	153,$\bar{2}$26,+	51.17

d (Å)	I	hkl	2θ(°)
1.778	6	135,160+	51.33
1.762	3	$\bar{3}33$	51.85
1.737	12	312	52.64
1.724	4	$\bar{1}17$	53.08
1.700	4	$\bar{2}45$	53.89
1.695	4	243	54.05
1.683	3	063,$\bar{3}$25	54.46
1.667	6	017,$\bar{1}$27	55.04
1.656	5	$\bar{3}41$	55.43
1.639	5	154,215	56.06
1.623	2	340,055	56.66
1.609	3	$\bar{3}$16,046	57.19
1.595	5	$\bar{3}$35,$\bar{2}$27	57.75
1.582	7	071,260	58.28
1.576	10	163,064	58.51
1.5619	2	$\bar{3}$26,$\bar{2}$46	59.10
1.5436	2	170,253,+	59.87
1.5231	2	$\bar{4}$13	60.76
1.5186	2	$\bar{1}$72,171	60.96
1.4995	3	$\bar{4}$04	61.82
1.4910	3	$\bar{3}$53,$\bar{3}$36	62.21
1.4757	5	$\bar{1}$65,008,+	62.93
1.4624	1	018,065	63.57
1.4493	1	$\bar{4}$24	64.21
1.4419	3	$\bar{3}27$	64.58
1.4344	1	$\bar{2}28$	64.96
1.4128	2	$\bar{1}38$	66.08
1.4058	4	$\bar{2}$65,$\bar{3}$46+	66.45
1.3885	3	081	67.39

Sample
The material was from the Specialty Chemicals Div. of Allied Chemical Corp., Morristown, N. J.

Color
Colorless

Optical data
Biaxial(-) $N\alpha$=1.43, $N\beta$=1.46, $N\gamma$=1.48, 2V is large.

Structure
Monoclinic, Aa(9),Z=4. The structure was determined by Pringle and Broadbent, [1965].

Lattice constants

	a(Å)	*b* (Å)	*c*(Å)	*β*(°)
NBS, sample at 25 °C	8.213 ±.001	7.812 ±.001	7.805 ±.001	120.04° ±.01

Density
(calculated) 2.124 g/cm³ at 25° C.

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

Additional patterns
1. PDF card 1-546 [Hanawalt et al.,1938]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2*θ*(°)
5.18	19	$\bar{1}11$	17.12
5.110	35	011	17.34
3.909	5	020	22.73
3.633	30	$\bar{2}11$	24.48
3.557	100	111,200	25.01
3.462	70	$\bar{2}02$	25.71
3.422	55	120	26.02
3.378	18	002	26.36
2.759	20	$\bar{1}22$	32.42
2.629	15	220	34.08
2.591	2	$\bar{2}22$	34.59
2.555	9	022	35.09
2.550		$\bar{3}11$	35.16
2.509	6	211	35.76
2.438	6	$\bar{1}31$	36.84
2.431	7	031	36.95
2.421	11	$\bar{1}13$	37.11
2.213	9	$\bar{3}13$	40.73
2.204	11	$\bar{3}22$	40.91
2.182	10	131	41.34
2.164	6	013	41.71
2.159	9	122	41.81
2.054	4	$\bar{4}02$	44.06
2.027	5	320	44.68
1.999	5	202	45.32
1.951	2	$\bar{2}04$	46.51
1.919	2	$\bar{4}11$	47.32
1.893	4	311	48.03
1.889	5	$\bar{4}13$	48.13
1.883	4	140	48.28
1.857	2	231	49.02
1.839	4	113	49.53
1.830	3	$\bar{2}33$	49.78
1.818	10	$\bar{4}22$	50.14
1.780	6	222	51.29
1.778	3	400	51.34
1.745	2	$\bar{2}24$	52.40
1.731	4	$\bar{4}04$	52.80
1.727	5	$\bar{3}33$	52.97
1.711	4	240	53.52

d (Å)	I	hkl	2θ(°)
1.703	6	033	53.78
1.690	8	042,004	54.24
1.685	6	$\bar{1}24$	54.42
1.618	2	420	56.85
1.591	3	$\bar{5}13$	57.93
1.576	1	$\bar{4}31,\bar{3}42$	58.51
1.561	2	331	59.12
1.550	2	024	59.59
1.527	1	$\bar{5}11$	60.58
1.523	1	051	60.77
1.5085	3	$\bar{5}22$	61.41
1.4803	1	322	62.71
1.4445	<1	$\bar{1}15$	64.45
1.4231	2	$\bar{5}24$	65.54
1.4145	3	$\bar{4}42$	65.99
1.3967	1	242	66.94
1.3879	2	124	67.42
1.3800	3	$\bar{2}44$	67.86
1.3605	2	$\bar{3}44$	68.97
1.3487	3	$\bar{6}02$	69.66
1.3455	2	251	69.85
1.3365	2	$\bar{5}31,520$	70.39
1.3315	2	015,$\bar{1}53$	70.69
1.3255	1	431	71.06
1.3146	1	440,313	71.74
1.2950	2	204	73.00
1.2802	2	160,$\bar{1}35$	73.98
1.2773	1	044	74.18
1.2724	1	$\bar{2}06$	74.51
1.2643	<1	$\bar{6}11$	75.07
1.2531	1	422,511	75.86
1.2351	<1	$\bar{1}62$	77.17
1.2294	<1	224	77.59
1.2266	1	$\bar{4}51$	77.80
1.2227	1	$\bar{5}35,260$	78.10
1.2197	2	351	78.33
1.2114	<1	$\bar{6}33$	78.97
1.2054	1	115	79.44
1.1868	<1	333	80.94
1.1758	1	$\bar{5}26$	81.86
1.1701	1	$\bar{3}62$	82.34
1.1632	<1	162	82.94

References

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

Pringle, G.E., and T.A. Broadbent (1965). Acta Cryst. 19, 426.

Sample

The sample was prepared by adding $FeCl_3$ solution to one containing NaF in HF.

Color

Colorless

Optical data

Almost isotropic, N≅1.41, very finely divided.

Structure

Monoclinic, Z=2 [Croft and Kestigian, 1968]. Space group $P2_1/n$ (14), by analogy with the powder pattern of cryolite, Na_3AlF_6.

Lattice constants

	a(Å)	b (Å)	c(Å)	β(°)
NBS, sample at 25 °C	5.513 ±.001	5.728 ±.001	7.964 ±.001	90.40 ±.01

Density

(calculated) 3.154 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 0.4$

Additional patterns

1. PDF card 1-0991 [Dow Chemical Co., Midland, Michigan]
2. PDF card 21-1125 [Croft and Kestigian 1968]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.65	75	011	19.07
4.54	45	$\bar{1}01$	19.52
4.52		101	19.62
3.98	100	002,110	22.34
3.56	9	$\bar{1}11$	24.98
3.55	8	111	25.04
2.864	35	020	31.20
2.819	95	$\bar{1}12$	31.72
2.806		112	31.87
2.756	25	200	32.46
2.542	6	120	35.28
2.484	20	210	36.13
2.424	25	$\bar{1}21$	37.06
2.398	15	$\bar{1}03$	37.47
2.384	40	103	37.70
2.376		$\bar{2}11$	37.83
2.326	4	022	38.67
2.212	11	$\bar{1}13$	40.76
2.202	16	113	40.95
2.146	15	$\bar{1}22$	42.07
2.139		122	42.21
2.115	4	$\bar{2}12$	42.72
1.987	85	220	45.62
1.947	6	023	46.61
1.929	6	$\bar{2}21$	47.07
1.925	4	221	47.18
1.857	3	031	49.00
1.838	7	$\bar{1}23$	49.54
1.804	17	130	50.54
1.792	10	$\bar{3}01$	50.91
1.780	25	$\bar{2}22$	51.28
1.776		114	51.40
1.760	16	$\bar{1}31$,131	51.91
1.750	5	310	52.22
1.722	2	032	53.16
1.707	4	311	53.65
1.643	30	$\bar{1}32$,132	55.90
1.634	25	024	56.24
1.619	7	$\bar{2}04$	56.81
1.606	45	$\bar{3}12$	57.32
1.598	25	312	57.64
1.547	7	320	59.74
1.541	8	$\bar{2}31$	60.00
1.535	9	015	60.25
1.519	6	$\bar{3}21$	60.93
1.5163	7	321,$\bar{3}03$	61.06
1.4908	4	133	62.22
1.4579	3	232	63.79
1.4318	4	040	65.09
1.4096	11	$\bar{2}24$,041	66.25
1.4023	10	224	66.64
1.3859	3	140	67.53
1.3782	3	400,034	67.96
1.3657	2	$\bar{1}41$,141	68.67

References

Croft, W.J. and M. Kestigian (1968). Mat. Res. Bull. 3, 571.

Sodium Selenate, Na_2SeO_4

Sample
The sample, obtained from K & K Laboratories, Inc., Plainview, N.Y., was recrystallized and dried at 50 °C.

Color
Colorless

Optical data
Biaxial(+), N_α=1.506, N_β=1.520, N_γ=1.534
2V is large.

Structure
Orthorhombic, Fddd (70), Z=8, isostructural with Na_2SO_4, form V (thenardite). The structure was determined by Náray-Szabó and Argay [1963] and refined by Kálmán and Cruickshank [1970].

Lattice constants

	a(Å)	*b*(Å)	*c*(Å)
NBS, sample at 25 °C--------	10.171 ±.001	12.587 ±.001	6.1038 ±.0003

Density
(calculated) 3.212 g/cm³ at 25° C.

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

Additional patterns
1. PDF card 1-272 [Hanawalt et al.,1938]
2. Náray-Szabó and Argay [1963]

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.831	100	111	18.35
3.959	45	220	22.44
3.273	70	131	27.22
3.150	45	040	28.31
2.884	90	311	30.98
2.746	55	022	32.58
2.618	5	202	34.22
2.543	1	400	35.26
2.421	25	331	37.10
2.418		222	37.15
2.012	8	242	45.01
1.978	10	440	45.83
1.940	2	260	46.79
1.918	35	351	47.37
1.865	16	422	48.78
1.801	2	133	50.63
1.753	2	531	52.13
1.728	30	062,313	52.95
1.700	1	171	53.87
1.659	2	442	55.33
1.6370	5	620,262	56.14
1.6104	12	333	57.15
1.5733	2	080	58.63
1.5635	5	153	59.03
1.5373	9	371	60.14
1.5258	3	004	60.64
1.4816	8	602	62.65
1.4336	6	353	65.00
1.4295	8	462,513	65.21
1.4237	5	224	65.51
1.4047	2	711	66.51
1.3729	6	044	68.26
1.3606	1	533	68.96
1.3510	2	191	69.52
1.3482	4	282	69.69
1.3396	13	731	70.20
1.3379	13	480	70.31
1.3360	11	173	70.42
1.3253	2	244	71.07
1.3184	7	660	71.50

d (Å)	I	hkl	2θ(°)
1.3152	7	571	71.70
1.3084	3	404	72.13
1.2814	1	424	73.90
1.2647	2	391	75.04
1.2523	2	373	75.92
1.2325	1	751	77.36
1.2218	1	2·10·0	78.17
1.2080	2	444	79.23
1.2065	2	115	79.35
1.1993	2	264	79.92
1.1774	2	713	81.72
1.1637	3	0·10·2	82.89
1.1537	1	822	83.77
1.1450	2	193	84.55
1.1440	2	315	84.65
1.1383	1	733	85.17
1.1346	1	2·10·2	85.51
1.1325	1	591	85.71
1.1181	3	1·11·1	87.09
1.1162	4	624	87.27
1.1076	5	335	88.13
1.0955	3	084	89.36
1.0920	3	155	89.72
1.0788	2	682	91.12
1.0741	1	931	91.63
1.0706	2	284	92.02
1.0678	2	3·11·1	92.34
1.0581	1	4·10·2	93.43
1.0491	1	0·12·0	94.49
1.0452	1	355	94.95

References

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

Kálmán, A. and D.W.J. Cruickshank (1970). Acta Cryst. B26, 436.

Náray-Szabó, I. and Gy. Argay (1963). Acta Chim. Hung. 39, 85.

Tin Sulfide (berndtite), beta, SnS_2

Sample

The sample was prepared by heating NH_4Cl, Sn amalgamated with Hg, and sulfur in excess until all the Hg was driven off. The remaining material was recrystallized by sublimation within an almost closed tube.

Major impurities

0.01 -0.1 % each: Al, Bi, Cd, Hg, and Pb

Color

Deep yellow brown

Structure

Hexagonal, $P\bar{3}m1$ (164), Z=1, isostructural with CdI_2 [Oftedal, 1928].

Lattice constants

	a(Å)	c(Å)
NBS, sample at 25 °C	3.6486 ±.0001	5.8992 ±.0003

Density

(calculated) 3.854 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.6$

Polymorphism

Moh [1969] found three additional lines in the pattern of this phase and concluded that it was of lower symmetry. Above 692 °C SnS_2 appears in a different crystal form (α). PDF card 21 -1231 [Guenter and Oswald, 1968] represents a polytype with c doubled which we did not observe.

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
5.89	100	001	15.02
3.162	30	100	28.20
2.951	5	002	30.26
2.784	55	101	32.12
2.155	25	102	41.88
1.9665	5	003	46.12
1.8240	30	110	49.96
1.7431	20	111	52.45
1.6693	8	103	54.96
1.5801	4	200	58.35
1.5521	4	112	59.51
1.5263	8	201	60.62
1.4749	4	004	62.97
1.3928	5	202	67.15
1.3374	6	113	70.33
1.2314	2	203	77.44
1.1942	2	210	80.33
1.1799	1	005	81.51
1.1705	5	211	82.31
1.1469	7	114	84.38
1.1069	5	212	88.20
1.1050	5	105	88.39
1.0778	<1	204	91.23
1.0534	4	300	93.98
1.0370	2	301	95.94
1.0208	3	213	97.98
0.9909	2	115	102.04
.9832	<1	006	103.15
.9454	1	205	109.13
.9385	1	106	110.33
.9285	2	303	112.12
.9121	2	220	115.24
.9015	2	221	117.39
.8762	1	310	123.06
.8715	<1	222	124.22
.8669	2	311	125.39
.8571	3	304	127.99
.8400	3	312	132.98
.8393	3	215	133.21

Additional patterns

1. Oftedal [1928]
2. PDF card 1-1010 [Hanawalt et al,1938]
3. Moh [1969]
4. Guenter and Oswald [1968]

References

Guenter, J.R. and H.R. Oswald (1968). Naturwiss. 55, 177.

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

Moh, G.H. (1969). Neues Jahrb. Mineral. Abhand. 111, 227.

Oftedal, I. (1928). Z. Physik. Chem.(Leipzig) 134, 301.

Sample

High-purity electrolytic vanadium crystals were obtained from the U.S. Bureau of Mines. The sample shipped in argon had the following Bureau of Mines analysis:

aluminum	10 ppm
carbon	16
chromium	<40
copper	< 5
hydrogen	42
manganese	5
nickel	6
nitrogen	10
oxygen	35
silicon	15

At NBS the crystals finer than 60 mesh were removed and annealed by R.M. Waterstrat for one minute at 1600 °C in a vacuum of 10^{-5} mm Hg using a thoria crucible. The sample was then mounted in silicone grease for x-ray measurements. Intensity values were obtained from fine powder of unknown oxygen content.

Color

Metallic silver

Structure

Cubic, Im3m (229), Z=2 [Hull, 1922].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	3.0274 ±.0001

Density

(calculated) 6.097 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 2.4$

Internal standard W, a = 3.16516 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
2.1411	100	110	42.17
1.5141	12	200	61.16
1.2363	19	211	77.08
1.0704	5	220	92.04
0.9575	8	310	107.12
.8739	3	222	123.63
.8091	11	321	144.37

Additional patterns

1. PDF card 1-1224, [Hanawalt et al., 1938]

References

Hanawalt, J.D., H.W. Rinn and L.K. Frevel, (1938). Ind. Eng. Chem. Anal.Ed. **10**,457.
Hull, A.W. (1922). Phys. Rev. **20**, 113.

Zinc Chromium Oxide, $ZnCr_2O_4$

Sample

Equimolar amounts of ZnO and Cr_2O_3 were mixed, pressed into pellets and heated to 900 °C for two hours. The pellets were ground, and reheated to sharpen the pattern.

Color

Light olive gray

Structure

Cubic, Fd3m (227), Z=8, spinel type, [Passerini, 1929].

Lattice constants

	a(Å)
NBS, sample at 25 °C----------	8.3275 ±.0001

Density

(calculated) 5.367 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 4.0$

Additional patterns

1. PDF card 21-1476[Kohlmuller and Omaly 1968].
2. PDF card 1-1123 [New Jersey Zinc Co. New Palmerton, Pa.]

Internal standard Ag, a = 4.08641 Å
CuKα_1 λ = 1.54056 Å; temp. 25 °C

d (Å)	I	hkl	2θ(°)
4.807	6	111	18.44
2.947	45	220	30.30
2.511	100	311	35.73
2.405	7	222	37.36
2.083	16	400	43.41
1.911	2	331	47.53
1.6996	13	422	53.90
1.6025	35	511	57.46
1.4719	40	440	63.11
1.4084	2	531	66.31
1.3168	5	620	71.60
1.2701	10	533	74.67
1.2558	4	622	75.67
1.2023	3	444	79.68
1.1664	2	711	82.66
1.1128	6	642	87.61
1.0840	12	731	90.57
1.0409	5	800	95.46
.9814	4	822	103.42
.9616	8	751	106.46
.9552	3	662	107.49
.9310	3	840	111.66
.8877	3	664	120.39
.8730	7	931	123.85
.8499	10	844	130.01
.8370	2	933	133.93
.8165	3	10·2·0	141.24
.8050	9	951	146.22
.8013	4	10·2·2	148.00

References

Kohlmuller, R.,and J. Omaly (1968). Bull. Soc. Chim. France 1968, 4383.

Passerini, L. (1929). Atti reale accad. nazl. Lincei 9, 338.

Zinc Iron Oxide (franklinite), $ZnFe_2O_4$

Sample

The sample was prepared by co-precipitation of the hydroxides, followed by heating at 600 °C for 17 hours and one hour at 800 °C.

Color

Medium brown

Optical data

Isotropic, N>2.00

Structure

Cubic, Fd3m (227), Z=8, spinel type, [Posnjak, 1930].

Lattice constants

	a(Å)
NBS, sample at 25 °C	8.4411 ±.0002

Density

(calculated) 5.324 g/cm³ at 25° C.

Reference intensity

$I/I_{corundum} = 3.8$

Additional patterns

1. PDF card 1-1108 [Posnjak, 1930]
2. PDF card 10-467 (natural mineral with Mn^{+2} and Fe^{+2}) [Ferguson, 1962]

Internal standard Ag, a = 4.08641 Å

$CuK\alpha_1$ λ = 1.54056 Å; temp. 25 °C

d (Å)	*I*	*hkl*	2θ(°)
4.873	7	111	18.19
2.984	35	220	29.92
2.543	100	311	35.26
2.436	6	222	36.86
2.109	17	400	42.84
1.937	<1	331	46.87
1.723	12	422	53.12
1.624	30	511	56.63
1.491	35	440	62.20
1.4270	1	531	65.34
1.3348	4	620	70.49
1.2872	9	533	73.51
1.2721	4	622	74.53
1.2184	2	444	78.43
1.1820	1	711	81.34
1.1280	5	642	86.14
1.0990	11	731	89.00
1.0553	4	800	93.76
0.9949	2	822	101.47
.9747	6	751	104.42
.9684	2	662	105.39
.9439	2	840	109.38
.8999	1	664	117.73
.8848	5	931	121.04
.8616	8	844	126.77
.8277	4	10·2·0	137.08
.8159	6	951	141.48
.8122	2	10·2·2	143.00

References

Ferguson, R.B. (1962). Geol. Soc. Am. Mem. 85, 193.

Posnjak, E. (1930). Am. J. Sci. 19, 67.

Structure
Monoclinic, C2/m (12), Z=4. The structure was determined by Ketelaar et al. [1947].

Lattice parameters
a=5.93±0.02, b=10.24±0.04, c=6.17±0.02Å, β=108° [ibid.]

Density
(calculated) 2.49 g/cm^3

Thermal parameters
Isotropic, overall B = 2.0

Atomic positions
Those used were the arrangement designated as the "ionic structure" [Ketelaar et al., 1947].

Scattering factors
Al°, Cl° [3.3.1A]

Scale factor
(integrated intensities) 1.811 x 10^4

Additional patterns
1. PDF card 1-1133[Hanawalt et al.,1938]
2. Laschkarew [1930]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
5.86	100	0 0 1	15.10
5.12	12	0 2 0	17.30
4.94	20	1 1 0	17.94
4.41	12	-1 1 1	20.10
3.86	6	0 2 1	23.04
3.36	2	1 1 1	26.52
2.93	30	0 0 2	30.44
2.92	19	1 3 0	30.54
2.89	1	-1 1 2	30.92
2.82	31	2 0 0	31.70
2.80	56	-1 3 1	31.94
2.462	96	1 3 1	36.46
2.445	50	-2 0 2	36.72
2.207	1	-2 2 2	40.86
2.084	1	2 2 1	43.38
1.956	1	0 0 3	46.38
1.929	2	0 4 2	47.08
1.922	11	1 3 2	47.26
1.907	6	-2 0 3	47.66
1.895	2	2 4 0	47.96
1.836	1	-3 1 2	49.60
1.787	1	-2 2 3	51.08
1.777	10	2 0 2 +	51.38
1.760	18	-1 3 3	51.90
1.710	20	-3 3 1	53.54
1.707	20	0 6 0	53.66
1.679	1	2 2 2	54.62
1.647	2	3 3 0	55.78
1.638	4	-3 3 2 +	56.10
1.517	2	1 3 3	61.04
1.506	1	-2 0 4	61.54
1.484	3	3 3 1	62.52
1.475	3	0 6 2	62.96
1.471	3	-3 3 3	63.14
1.467	4	0 0 4	63.34
1.460	3	2 6 0 +	63.68
1.420	1	-4 2 1	65.68
1.415	2	2 0 3	65.94
1.410	4	4 0 0	66.22
1.404	5	-1 3 4	66.54
1.400	8	-2 6 2	66.78
1.284	1	4 0 1	73.74
1.272	1	-2 6 3	74.56
1.231	3	2 6 2	77.48
1.223	1	-4 0 4	78.10
1.174	1	0 0 5	82.04
1.119	2	3 3 3	86.98
1.112	2	0 6 4 +	87.64
1.108	2	-3 3 5 +	88.08
1.089	1	2 6 3	90.00
1.087	2	4 6 0	90.26
1.084	3	1 9 1	90.60
1.083	2	-5 3 3	90.70
1.081	2	-4 0 5	90.88
1.003	1	5 3 1	100.36
.995	1	-1 9 3	101.40
.994	1	-4 6 4	101.60
.988	1	-6 0 2	102.42
.986	1	-3 9 1	102.74
.972	1	3 3 4	104.76
.967	1	0 6 5	105.60
.963	1	-3 3 6	106.22

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			$2\theta(°)$ $\lambda = 1.54056$ Å
5.87	83	0	0	1	15.09
5.12	10	0	2	0	17.31
4.94	17	1	1	0	17.94
4.41	10	-1	1	1	20.10
3.86	5	0	2	1	23.03
3.36	2	1	1	1	26.52
2.93	29	0	0	2	30.44
2.92	5	1	3	0	30.59
2.92	1	-2	0	1	30.61
2.89	1	-1	1	2	30.92
2.82	30	2	0	0	31.70
2.80	57	-1	3	1	31.95
2.462	100	1	3	1	36.47
2.445	48	-2	0	2	36.72
2.207	1	-2	2	2	40.86
2.084	2	2	2	1	43.39
1.956	1	0	0	3	46.38
1.929	2	0	4	2	47.07
1.925	1	1	5	0	47.17
1.922	12	1	3	2	47.26
1.907	7	-2	0	3	47.66
1.895	1	2	4	0	47.96
1.836	2	-3	1	2	49.61
1.787	1	-2	2	3	51.07
1.777	12	2	0	2	51.37
1.774	2	1	5	1	51.45
1.761	22	-1	3	3	51.89
1.710	24	-3	3	1	53.53
1.707	12	0	6	0	53.66
1.703	1	2	4	1	53.78
1.679	1	2	2	2	54.62
1.647	2	3	3	0	55.78
1.639	3	0	6	1	56.07
1.638	3	-3	3	2	56.12
1.517	2	1	3	3	61.04
1.506	1	-2	0	4	61.53
1.484	3	3	3	1	62.52
1.475	3	0	6	2	62.95
1.471	3	-3	3	3	63.15
1.467	4	0	0	4	63.35
1.460	3	2	6	0	63.68
1.459	2	-4	0	2	63.74
1.421	1	-4	2	1	65.67
1.415	3	2	0	3	65.94
1.410	5	4	0	0	66.23
1.404	6	-1	3	4	66.54
1.402	1	-1	7	1	66.68
1.400	9	-2	6	2	66.79
1.379	1	-3	5	2	67.89
1.284	1	4	0	1	73.74
1.272	2	-2	6	3	74.56
1.234	1	1	3	4	77.24
1.231	5	2	6	2	77.47
1.223	2	-4	0	4	78.10
1.174	2	0	0	5	82.04
1.119	2	3	3	3	86.98
1.113	1	-5	3	1	87.61
1.112	2	0	6	4	87.64
1.109	1	-4	6	2	87.99
1.108	1	-1	9	1	88.07
1.108	2	-3	3	5	88.10
1.089	2	2	6	3	89.99
1.087	3	4	6	0	90.25
1.084	3	1	9	1	90.61
1.083	3	-5	3	3	90.71
1.081	1	-4	0	5	90.88
1.033	1	1	3	5	96.40
1.026	1	4	6	1	97.32
1.022	1	1	9	2	97.82
1.019	1	-5	3	4	98.21
1.003	2	5	3	1	100.36
.995	2	-1	9	3	101.40
.994	2	-4	6	4	101.60
.988	1	-6	0	2	102.42
.986	2	-3	9	1	102.73
.972	2	3	3	4	104.77
.967	2	0	6	5	105.60
.963	2	-3	3	6	106.22
.923	1	5	3	2	113.20
.915	1	-1	9	4	114.63
.913	1	-4	6	5	115.00

Reference

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

Ketelaar, J.A.A., C.H.MacGillavry,and P.A. Renes (1947). Rec. Trav. Chim. 66, 501.

Laschkarew, W.E. (1930). Z. Anorg. u. allgem. Chem. 193, 270.

Structure
Cubic, Fm3m (225), Z=4 [Gerlach, 1922]

Lattice parameters
a=5.5393Å, (published value: a=5.53912± 0.00013Å)[Zollweg, 1955]

Density
(calculated) 5.992 g/cm^3

Thermal parameters
Overall temperature factor, 1.0

Scattering factors
Ba^{+2} [Cromer and Waber, 1965]
O^{-2} [Suzuki, 1960]

Scale factor
[integrated intensities] 6.438 × 10^4

Additional patterns
1. PDF 1-746 [Hanawalt et al., 1938]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.1974	100	1 1 1	27.88
2.7693	86	2 0 0	32.30
1.9585	49	2 2 0	46.32
1.6704	32	3 1 1	54.92
1.5989	14	2 2 2	57.60
1.3847	5	4 0 0	67.60
1.2708	10	3 3 1	74.62
1.2387	12	4 2 0	76.90
1.1307	8	4 2 2	85.88
1.0660	6	5 1 1 +	92.54
.9792	2	4 4 0	103.74
.9364	5	5 3 1	110.70
.9232	5	4 4 2 +	113.10
.8758	4	6 2 0	123.16
.8448	3	5 3 3	131.52
.8351	4	6 2 2	134.56
.7996	1	4 4 4	148.90

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
3.1981	100	1 1 1	27.87
2.7697	89	2 0 0	32.30
1.9584	58	2 2 0	46.32
1.6702	43	3 1 1	54.93
1.5991	18	2 2 2	57.59
1.3848	8	4 0 0	67.59
1.2708	16	3 3 1	74.62
1.2386	20	4 2 0	76.91
1.1307	15	4 2 2	85.88
1.0660	9	5 1 1	92.53
1.0660	3	3 3 3	92.53
.9792	5	4 4 0	103.74
.9363	14	5 3 1	110.71
.9232	2	6 0 0	113.10
.9232	10	4 4 2	113.10
.8758	10	6 2 0	123.16
.8447	8	5 3 3	131.53
.8351	11	6 2 2	134.56
.7995	5	4 4 4	148.91

Reference
Cromer, D.T. and J. T. Waber (1965). Acta Cryst. 18, 104.
Gerlach, W. (1922). Z. Physik 9, 184.
Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem. Anal. Ed.10,457.
Suzuki, T. (1960). Acta Cryst. 13, 279.
Zollweg, R.J. (1955). Phys.Rev.100 #2,671.

Structure

Hexagonal, Z=2, isostructural with magnesium [McKeehan, 1922]. $P6_3/mmc$ (194) [Neuberger, 1932].

Lattice parameters

a= 2.2859 ±.0002, c= 3.5844±.0003Å, (published values: a=2.2858 ±.0002, c=3.5843 ±.0003Å) [McKay and Hill, 1963].

Density

(calculated) 1.845 g/cm^3

Thermal parameters

Isotropic, overall B = 2.0

Polymorphism

A second hexagonal modification of beryllium exists. It has different alloying properties and a volume 29% larger than the one described here [Sidhu and Henry, 1950].

Scattering factors

Be^0 [3.3.1A]

Scale factor

(integrated intensities) 5.998

Additional patterns

1. PDF card 1-1291[Hanawalt et al.,1938]
2. Jaeger and Zanstra [1933]

Reference

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

Jaeger, F.M. and J.E. Zanstra(1933). Proc. Acad. Sci. Amsterdam 36, 636.

McKay, K.J.H. and N.A. Hill(1963). J.Nucl. Materials 8, 263.

McKeehan, L.W. (1922). Proc.Natl.Acad.Sci. US 8, 270.

Neuberger, M.C.(1932). Z. Phys. Chem. B17, 285.

Sidhu, S.S. and C.O. Henry(1950). J. Appl. Phys. 21, 1036.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(°)$ λ = 1.54056 Å
1.9795	30	1 0 0	45.80
1.7925	25	0 0 2	50.90
1.7330	100	1 0 1	52.78
1.3287	9	1 0 2	70.86
1.1430	9	1 1 0	84.74
1.0230	8	1 0 3	97.70
.9898	1	2 0 0	102.20
.9636	8	1 1 2	106.14
.9541	6	2 0 1	107.68
.8961	1	0 0 4	118.54
.8664	1	2 0 2	125.50
.8163	1	1 0 4	141.32

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ λ = 1.54056 Å
1.9797	23	1 0 0	45.80
1.7922	25	0 0 2	50.91
1.7329	100	1 0 1	52.78
1.3286	11	1 0 2	70.87
1.1429	12	1 1 0	84.74
1.0229	12	1 0 3	97.70
.9898	2	2 0 0	102.19
.9637	14	1 1 2	106.13
.9541	10	2 0 1	107.67
.8961	2	0 0 4	118.54
.8665	3	2 0 2	125.50
.8164	3	1 0 4	141.31

Beryllium Lanthanum Oxide, $Be_2La_2O_5$

Structure

Monoclinic, C2/c (15), Z=4 [Harris and Yakel, 1968]

Lattice parameters

a= 7.5356 ± 0.0006, b= 7.3476 ± 0.0017, c= 7.4387 ± 0.0006Å, β= 91°33′±1′[ibid.]

Density

(calculated) 6.061 g/cm^3 [ibid.]

Thermal parameters

Isotropic: La 0.414
Be 0.412
O(1) 0.564
O(2) 0.480
O(3) 0.404
O(4) 0.666

Scattering factors

La^{3+} [Cromer and Waber, 1965], corrected for dispersion using $\Delta f'=2.6$, $\Delta f''=9.2$
Be^{2+} [Cromer and Waber]
O^- [3.3.1A]

Scale factor

(integrated intensities) 11.38 × 10^4

Additional patterns

1. Weir and Van Valkenburg [1960].

Reference

Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Harris, L.A. and H.L. Yakel (1968). Acta Cryst. B24, 672.
Weir, C.E. and A. Van Valkenburg [1960]. J. Res. Natl. Bur. Std. 64A, 105.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.260	2	1 1 0	16.84
4.255	4	1 1 1	20.86
3.767	100	2 0 0	23.60
3.717	54	0 0 2	23.92
3.675	73	0 2 0	24.20
3.292	21	0 2 1	27.06
3.064	34	-1 1 2	29.12
3.009	67	1 1 2	29.66
2.682	30	-2 0 2	33.38
2.630	79	2 2 0	34.06
2.612	70	0 2 2 +	34.30
2.494	24	-2 2 1	35.98
2.465	8	2 2 1	36.42
2.376	6	3 1 0	37.84
2.259	1	-1 1 3	39.88
2.227	11	1 1 3 +	40.48
2.220	7	1 3 1	40.60
2.166	47	-2 2 2	41.66
2.128	24	2 2 2	42.44
2.054	5	0 2 3	44.04
2.026	12	-3 1 2	44.70
1.980	25	3 1 2 +	45.80
1.967	17	1 3 2	46.12
1.883	17	4 0 0	48.28
1.859	2	0 0 4	48.96
1.837	8	0 4 0	49.58
1.821	2	-2 2 3	50.04
1.7834	16	0 4 1	51.18
1.7634	26	-1 1 4	51.80
1.7422	20	1 1 4	52.48
1.7379	12	-3 1 3	52.62
1.7043	5	-1 3 3	53.74
1.6990	14	-4 0 2 +	53.92
1.6938	8	3 1 3	54.10
1.6903	6	1 3 3	54.22
1.6857	4	-2 0 4	54.38
1.6761	14	4 2 0	54.72
1.6621	3	4 0 2	55.22
1.6510	7	2 4 0	55.62
1.6467	8	0 4 2	55.78
1.6434	5	-4 2 1	55.90
1.6263	4	4 2 1	56.54
1.6159	8	-2 4 1	56.94
1.6076	10	2 4 1	57.26
1.5974	2	-3 3 2	57.66
1.5745	5	3 3 2	58.58
1.5420	9	-4 2 2	59.94
1.5318	1	-2 2 4	60.38
1.5154	6	-2 4 2 +	61.10
1.5021	2	2 4 2	61.70

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.4827	8	-3 1 4	62.60
1.4759	3	0 4 3 +	62.92
1.4589	6	-1 3 4	63.74
1.4463	15	3 1 4 +	64.36
1.4431	9	-3 3 3	64.52
1.4189	4	3 3 3	65.76
1.4147	3	1 5 1	65.98
1.4041	1	-4 2 3	66.54
1.3818	3	-2 4 3	67.76
1.3665	1	2 4 3	68.62
1.3596	7	5 1 2	69.02
1.3413	2	-4 0 4 +	70.10
1.3149	5	4 4 0	71.72
1.3067	1	0 4 4	72.24
1.2990	5	-4 4 1	72.74
1.2907	2	4 4 1	73.28
1.2877	5	-3 3 4	73.48
1.2841	2	5 3 0	73.72
1.2755	1	-3 1 5	74.30
1.2636	5	3 3 4	75.12
1.2599	5	5 3 1 +	75.38
1.2582	4	-1 3 5	75.50
1.2553	5	6 0 0	75.70
1.2492	6	-1 5 3 +	76.14
1.2472	5	-4 4 2 +	76.28
1.2439	6	1 5 3	76.52
1.2404	2	0 0 6	76.78
1.2115	4	-1 1 6	78.96
1.2084	7	0 6 1	79.20
1.2049	4	5 3 2	79.48
1.2013	6	1 1 6	79.76
1.1993	4	-6 0 2	79.92
1.1961	2	3 5 2	80.18
1.1880	3	6 2 0	80.84
1.1779	1	-6 2 1	81.68
1.1743	1	0 2 6	81.98
1.1710	5	-5 1 4 +	82.26
1.1680	4	2 0 6	82.52
1.1521	4	-2 6 1	83.92
1.1492	6	2 6 1 +	84.18
1.1450	2	-3 3 5	84.56
1.1412	6	5 1 4 +	84.90
1.1402	6	-6 2 2	85.00
1.1371	3	1 5 4	85.28
1.1354	3	-3 5 3	85.44
1.1290	1	5 3 3	86.04
1.1230	4	3 5 3 +	86.62
1.1129	1	2 2 6	87.60
1.1105	4	-3 1 6	87.84
1.1079	2	2 6 2	88.10

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.260	2	1 1 0	16.84
4.256	4	1 1 1	20.85
3.766	100	2 0 0	23.60
3.718	52	0 0 2	23.91
3.674	75	0 2 0	24.21
3.294	23	0 2 1	27.05
3.063	37	-1 1 2	29.13
3.009	72	1 1 2	29.66
2.683	33	-2 0 2	33.37
2.630	87	2 2 0	34.06
2.613	54	0 2 2	34.29
2.611	32	2 0 2	34.32
2.494	27	-2 2 1	35.98
2.465	8	2 2 1	36.42
2.376	8	3 1 0	37.83
2.259	1	-1 1 3	39.88
2.228	6	-1 3 1	40.45
2.226	9	1 1 3	40.49
2.217	4	1 3 1	40.65
2.166	58	-2 2 2	41.65
2.128	29	2 2 2	42.44
2.055	6	0 2 3	44.03
2.026	15	-3 1 2	44.70
1.981	9	-1 3 2	45.76
1.979	27	3 1 2	45.81
1.966	21	1 3 2	46.12
1.883	23	4 0 0	48.29
1.859	2	0 0 4	48.96
1.837	11	0 4 0	49.59
1.821	2	-2 2 3	50.05
1.7833	20	0 4 1	51.18
1.7632	35	-1 1 4	51.81
1.7533	1	3 3 0	52.12
1.7424	27	1 1 4	52.47
1.7376	1	-3 1 3	52.63
1.7045	6	-1 3 3	53.73
1.6993	5	3 3 1	53.91
1.6986	13	-4 0 2	53.93
1.6937	1	3 1 3	54.10
1.6903	6	1 3 3	54.22
1.6852	2	-2 0 4	54.40
1.6759	19	4 2 0	54.73
1.6620	3	4 0 2	55.22
1.6510	9	2 4 0	55.62
1.6469	6	0 4 2	55.77
1.6434	4	-4 2 1	55.90
1.6265	5	4 2 1	56.53
1.6158	11	-2 4 1	56.94
1.6077	13	2 4 1	57.25
1.5975	2	-3 3 2	57.66

Beryllium Lanthanum Oxide, $Be_2La_2O_5$ – continued

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.5744	7	3 3 2	58.58
1.5418	13	-4 2 2	59.95
1.5317	2	-2 2 4	60.38
1.5156	6	-2 4 2	61.09
1.5142	5	4 2 2	61.15
1.5023	2	2 4 2	61.69
1.4826	12	-3 1 4	62.60
1.4759	1	5 1 0	62.92
1.4758	2	0 4 3	62.92
1.4589	9	-1 3 4	63.74
1.4471	10	1 3 4	64.32
1.4463	16	3 1 4	64.36
1.4443	2	-3 3 3	64.46
1.4188	5	3 3 3	65.76
1.4146	2	1 5 1	65.99
1.4041	1	-4 2 3	66.54
1.3817	4	-2 4 3	67.77
1.3666	2	2 4 3	68.61
1.3594	11	5 1 2	69.03
1.3424	2	1 5 2	70.04
1.3413	3	-4 0 4	70.10
1.3150	8	4 4 0	71.72
1.3066	1	0 4 4	72.25
1.2991	7	-4 4 1	72.73
1.2907	3	4 4 1	73.28
1.2877	6	-3 3 4	73.48
1.2832	1	5 3 0	73.78
1.2754	1	-3 1 5	74.31
1.2636	8	3 3 4	75.12
1.2599	2	-4 2 4	75.38
1.2597	2	5 3 1	75.39
1.2582	5	-1 3 5	75.49
1.2555	4	6 0 0	75.69
1.2494	6	-1 5 3	76.12
1.2487	3	1 3 5	76.17
1.2474	2	3 5 1	76.27
1.2471	3	-4 4 2	76.29
1.2438	6	1 5 3	76.53
1.2393	1	0 0 6	76.86
1.2324	1	4 4 2	77.37
1.2114	7	-1 1 6	78.97
1.2083	8	0 6 1	79.21
1.2045	4	5 3 2	79.51
1.2012	8	1 1 6	79.77
1.1994	4	-6 0 2	79.92
1.1954	1	3 5 2	80.24
1.1880	5	6 2 0	80.84
1.1778	1	-6 2 1	81.69
1.1743	2	0 2 6	81.98
1.1711	6	-5 1 4	82.26

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.1708	3	-4 4 3	82.28
1.1679	2	2 0 6	82.53
1.1520	7	-2 6 1	83.92
1.1504	1	-5 3 3	84.06
1.1491	6	2 6 1	84.19
1.1449	3	-3 3 5	84.57
1.1424	2	-1 5 4	84.79
1.1412	7	5 1 4	84.90
1.1401	8	-5 2 2	85.00
1.1367	1	1 5 4	85.32
1.1354	4	-3 5 3	85.44
1.1290	2	5 3 3	86.04
1.1237	3	3 3 5	86.55
1.1233	2	6 2 2	86.58
1.1229	5	3 5 3	86.63
1.1130	1	2 2 6	87.59
1.1106	7	-3 1 6	87.83
1.1087	1	2 6 2	88.02
1.0979	2	0 6 3	89.11
1.0979	4	-1 3 6	89.11
1.0903	3	1 3 6	89.90
1.0875	4	3 1 6	90.20
1.0832	1	-4 4 4	90.65
1.0822	1	-6 2 3	90.76
1.0676	3	-5 3 4	92.36
1.0648	2	7 1 0	92.68
1.0574	2	-2 6 3	93.51
1.0544	1	-3 5 4	93.86
1.0537	1	-6 0 4	93.94
1.0507	1	2 6 3	94.30
1.0449	3	5 3 4	94.99
1.0411	2	3 5 4	95.44
1.0389	2	5 5 1	95.71
1.0381	4	-1 5 5	95.81
1.0365	2	6 4 0	96.00
1.0327	6	1 5 5	96.47
1.0301	1	-1 7 1	96.79
1.0297	4	-6 4 1	96.84
1.0291	1	1 7 1	96.92
1.0274	1	0 4 6	97.14
1.0235	2	6 4 1	97.64
1.0226	2	4 0 6	97.74
1.0211	4	-3 3 6	97.93
1.0190	5	-4 6 1	98.21
1.0164	4	7 1 2	98.55
1.0150	4	4 6 1	98.74
1.0129	2	-6 2 4	99.01
1.0072	1	5 5 2	99.77
1.0042	2	-6 4 2	100.17
1.0031	2	3 3 6	100.33

Structure

Cubic, Fm3m (225),Z=4. The structure was determined by Hull [1921].

Lattice parameters

a = 5.5886 ± .0002Å, (published value: a = 5.5884 ±.0002Å) [Bernstein and Smith 1959].

Density

(calculated) 1.525 g/cm^3

Thermal parameters

Isotropic, overall B=2.0

Scattering factors

Ca° [3.3.1A]

Scale factor

(integrated intensities) 0.9867 x 10^4

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ λ = 1.54056 Å
3.2269	100	1	1	1		27.62
2.7945	46	2	0	0		32.00
1.9754	23	2	2	0		45.90
1.6851	23	3	1	1		54.40
1.6133	6	2	2	2		57.04
1.3971	2	4	0	0		66.92
1.2820	6	3	3	1		73.86
1.2498	5	4	2	0	+	76.10
1.1408	3	4	2	2		84.94
1.0755	3	5	1	1	+	91.48
.9880	1	4	4	0		102.46
.9446	2	5	3	1	+	109.26
.9314	1	4	4	2		111.58
.8836	1	6	2	0	+	121.32
.8523	1	5	3	3		129.32
.8425	1	6	2	2		132.20
.7825	2	7	1	1	+	159.68

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*			$2\theta(°)$ λ = 1.54056 Å
3.2266	100	1	1	1	27.62
2.7943	48	2	0	0	32.00
1.9759	28	2	2	0	45.89
1.6850	30	3	1	1	54.40
1.6133	3	2	2	2	57.04
1.3971	3	4	0	0	66.92
1.2821	9	3	3	1	73.85
1.2497	4	4	2	0	76.11
1.2497	4	0	2	4	76.11
1.1408	5	4	2	2	84.94
1.0755	4	5	1	1	91.48
1.0755	1	3	3	3	91.48
.9879	1	4	4	0	102.46
.9447	3	5	3	1	109.26
.9447	3	1	3	5	109.26
.9314	3	4	4	2	111.58
.8836	1	0	2	6	121.32
.8836	1	6	2	0	121.32
.8523	2	5	3	3	129.33
.8425	2	6	2	2	132.20
.8066	1	4	4	4	145.46
.7826	4	7	1	1	159.67
.7826	4	5	5	1	159.67

Additional patterns

1. PDF card 1-735 [Hanawalt et al.,1938]
2. Hull [1921]

Reference

Bernstein,B.T. and J.F. Smith (1959). Acta Cryst. 12, 419.

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

Hull, A.W. (1921). Phys. Rev. 17, 42.

Cesium Beryllium Fluoride, $CsBeF_3$

Structure

Orthorhombic, Pnma (62), Z=4 [Steinfink and Brunton, 1968]

Lattice parameters

a=4.828±.002,b=6.004±.002,c=12.794±.003Å [ibid.]

Density

(calculated) 3.55 g/cm^3 [ibid.]

Thermal parameters

Isotropic: Cs 2.62
F(1) 4.22
F(2) 4.39
Be 2.44

Polymorphism

Breusov, Novoselova, and Simanov [1958] described three phases, specifying that the beta phase occurred between 140 and 360 °C. The material being described here was thought to be the beta form, [Steinfink and Brunton,1968]

Scattering factors

Be^{2+}, F^- [Cromer and Waber,1965]
Cs^+ [ibid.], corrected for dispersion by $\Delta f'$=-1.40 and $\Delta f''$=7.75 [Cromer,1965]

Scale factor

(integrated intensities) 7.513 × 10^4

Additional patterns

1. PDF 17-323 (at 200 °C). [Breusov and Simanov,1959]

References

Breusov, O.N., A.V. Novoselova, and Yu.P. Simanov (1958). Dokl. Akad. Nauk. S.S.S.R. 118, 935.

Breusov, O.N. and Yu. P. Simanov (1959). Russ. J. Inorg. Chem. 4, 1190.

Cromer, D.T. (1965). Acta Cryst. 18, 17.

Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.

Steinfink, H. and G.D. Brunton(1968). Acta Cryst. B24, 807.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ*(°) λ = 1.54056 Å
5.433	28	0 1 1	16.30
3.854	37	1 0 2	23.06
3.610	100	1 1 1	24.64
3.477	64	0 1 3	25.60
3.243	3	1 1 2	27.48
3.197	30	0 0 4	27.88
3.002	17	0 2 0	29.74
2.822	13	1 1 3	31.68
2.667	4	1 0 4	33.58
2.414	16	2 0 0	37.22
2.368	55	1 2 2	37.96
2.259	1	2 0 2	39.88
2.239	1	2 1 0	40.24
2.206	8	2 1 1	40.88
2.189	4	0 2 4	41.20
2.132	3	0 0 6	42.36
2.116	27	1 1 5	42.70
2.101	2	2 0 3	43.02
1.994	4	1 2 4	45.46
1.983	13	2 1 3	45.72
1.978	10	0 3 1	45.84
1.951	2	1 0 6	46.52
1.927	10	2 0 4	47.12
1.881	4	2 2 0	48.34
1.829	5	1 3 1	49.80
1.812	8	0 3 3	50.32
1.748	5	0 1 7	52.28
1.738	2	0 2 6	52.60
1.696	1	1 3 3	54.02
1.635	6	1 2 6	56.20
1.622	3	2 2 4	56.72
1.598	2	2 0 6 +	57.62
1.561	1	3 0 2	59.14
1.543	4	3 1 1	59.90
1.529	3	2 3 1	60.48
1.518	2	1 0 8	60.98
1.501	3	0 4 0	61.76
1.499	4	1 3 5	61.86
1.461	1	3 1 3	63.66
1.449	4	2 3 3	64.22
1.416	3	2 1 7	65.90
1.411	2	2 2 6	66.18
1.399	2	1 4 2	66.84
1.385	4	3 2 2	67.60
1.359	1	0 4 4	69.06
1.355	3	1 2 8	69.30
1.350	2	0 3 7	69.60
1.333	1	2 0 8	70.58
1.330	3	1 1 9	70.80
1.329	3	3 1 5	70.86

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.275	1	2 4 0	74.36
1.248	1	3 3 1	76.22
1.184	1	2 4 4	81.16
1.181	2	3 2 6	81.42
1.178	3	2 3 7 +	81.66
1.160	1	1 5 1	83.18
1.140	1	4 1 3	84.98
1.129	1	4 0 4	86.02
1.126	1	3 3 5 +	86.30
1.060	1	1 5 5 +	93.16
1.058	1	2 2 10 +	93.46
1.049	1	3 1 9	94.50
.901	1	1 5 9	117.52
.901	1	3 5 5	117.54

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.435	24	0 1 1	16.29
3.854	35	1 0 2	23.06
3.610	100	1 1 1	24.64
3.477	64	0 1 3	25.60
3.243	2	1 1 2	27.48
3.199	32	0 0 4	27.87
3.002	18	0 2 0	29.74
2.821	14	1 1 3	31.69
2.666	4	1 0 4	33.58
2.414	18	2 0 0	37.22
2.368	62	1 2 2	37.96
2.354	1	0 1 5	38.20
2.259	1	2 0 2	39.88
2.240	1	2 1 0	40.23
2.206	10	2 1 1	40.87
2.189	5	0 2 4	41.21
2.132	3	0 0 6	42.35
2.116	31	1 1 5	42.70
2.101	1	2 0 3	43.02
1.994	4	1 2 4	45.46
1.983	15	2 1 3	45.72
1.977	3	0 3 1	45.85
1.951	2	1 0 6	46.52
1.927	13	2 0 4	47.13
1.881	5	2 2 0	48.34
1.830	7	1 3 1	49.79
1.812	10	0 3 3	50.32
1.748	6	0 1 7	52.28
1.738	2	0 2 6	52.60
1.696	1	1 3 3	54.01
1.636	8	1 2 6	56.19
1.622	4	2 2 4	56.72
1.599	1	0 0 8	57.59
1.598	2	2 0 6	57.63
1.561	2	3 0 2	59.15
1.543	5	3 1 1	59.89
1.530	4	2 3 1	60.47
1.518	3	1 0 8	60.98
1.510	1	3 1 2	61.32
1.501	3	0 4 0	61.75
1.499	5	1 3 5	61.86
1.460	2	3 1 3	63.66
1.449	5	2 3 3	64.22
1.416	5	2 1 7	65.91
1.411	2	2 2 6	66.19
1.399	3	1 4 2	66.83
1.385	5	3 2 2	67.60
1.359	2	0 4 4	69.07
1.355	4	1 2 8	69.30
1.350	3	0 3 7	69.60
1.333	1	2 0 8	70.59
1.330	3	1 1 9	70.79
1.329	3	3 1 5	70.87
1.297	1	3 2 4	72.89
1.279	1	0 0 10	74.04
1.275	2	2 4 0	74.36
1.248	1	3 3 1	76.21
1.190	1	1 4 6	80.71
1.184	2	2 4 4	81.16
1.181	2	3 2 6	81.42
1.178	1	4 1 1	81.65
1.178	3	2 3 7	81.67
1.177	1	0 2 10	81.76
1.160	2	1 5 1	83.17
1.156	1	0 5 3	83.58
1.143	1	1 2 10	84.70
1.140	1	4 1 3	84.99
1.130	1	2 0 10	85.91
1.129	1	4 0 4	86.02
1.127	1	1 3 9	86.24
1.126	1	3 3 5	86.31
1.082	1	3 4 2	90.80
1.067	1	1 4 8	92.38
1.061	1	3 2 8	93.09
1.060	2	1 5 5	93.16
1.058	1	2 2 10	93.46
1.057	1	4 2 4	93.57
1.049	1	3 1 9	94.49
1.043	1	2 5 3	95.27
1.032	1	2 1 11	96.53
1.005	1	4 3 3	100.14
.993	1	4 1 7	101.69
.984	1	1 2 12	103.09
.969	1	1 6 2	105.37
.960	1	3 5 1	106.76

Structure

Monoclinic, $P2_1/a(14)$, Z=12 [Zachariasen, 1963].

Lattice parameters

a=7.122±.002, b=8.842±.002, c=6.771±.002Å, β=93.26±.01° [ibid.]

Density

(calculated) 2.051 g/cm³ [ibid.]

Thermal parameters

Isotropic:

B_I	0.72
B_{II}	1.06
B_{III}	0.98
O_I	1.01
O_{II}	0.89
O_{III}	1.11
O_{IV}	1.09
O_V	1.23
O_{VI}	1.15
H_I	2.50
H_{II}	2.50
H_{III}	2.50

Polymorphism

There are two other polymorphs of HBO_2. One form is orthorhombic [Tazaki, 1940], and the other, cubic [Zachariasen, 1963]. PDF cards 9-15 and 15-403 appear to be the orthorhombic form. PDF card 15-868 contains the pattern of the cubic form.

Scattering factors

H^0, B^0 [McWeeny, 1951]
O^0 [Berghuis et al., 1955]

Scale factor

(integrated intensities) 1.116×10^4

Reference

Berghuis, J., IJ. M. Haanapel, M. Potters, B.O. Loopstra, C.H. MacGillavry, and A. L. Veenendaal (1955). Acta Cryst. 8,478.
McWeeny, R. (1951). Acta Cryst. 13, 403.
Tazaki, H. (1940). J.Sci.Hiroshima U.A10,37.
Zachariasen, W.H. (1963). Acta Cryst. 16, 385.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
6.753	33	0 0 1	13.10
5.542	1	1 1 0	15.98
5.368	7	0 1 1	16.50
4.380	22	1 1 -1	20.26
4.195	100	1 1 1	21.16
3.556	5	2 0 0	25.02
3.324	5	1 2 -1	26.80
3.297	9	2 1 0	27.02
3.241	10	1 2 1	27.50
3.222	10	2 0 -1	27.66
3.157	3	0 1 2	28.24
3.074	100	2 0 1	29.02
3.027	2	2 1 -1	29.48
2.944	1	1 1 -2	30.34
2.831	2	1 1 2	31.58
2.723	7	1 3 0	32.86
2.701	10	0 3 1	33.14
2.685	10	0 2 2	33.34
2.550	11	1 2 -2	35.16
2.545	9	1 3 -1	35.24
2.524	12	2 2 1 +	35.54
2.425	6	2 1 -2	37.04
2.383	1	2 0 2	37.72
2.301	1	2 1 2	39.12
2.290	2	3 1 0	39.32
2.211	10	0 4 0	40.78
2.206	8	3 1 -1	40.88
2.190	17	2 2 -2	41.18
2.144	3	1 3 -2	42.12
2.128	3	2 3 1	42.44
2.111	2	1 4 0	42.80
2.025	2	3 2 -1	44.72
2.008	15	0 2 3 +	45.12
1.958	6	1 2 -3	46.32
1.916	1	2 3 -2	47.40
1.907	3	1 2 3 +	47.64
1.849	10	3 1 2 +	49.24
1.818	1	3 2 -2	50.14
1.802	4	3 3 -1	50.60
1.795	4	2 4 1	50.82
1.791	3	0 3 3	50.96
1.778	2	4 0 0 +	51.36
1.762	1	3 3 1	51.84
1.717	2	1 3 3 +	53.32
1.711	3	4 1 -1	53.52
1.696	2	4 0 1	54.04
1.665	1	4 1 1	55.10
1.658	3	1 5 1	55.36
1.652	3	3 1 -3 +	55.58
1.622	1	4 2 -1	56.70

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.617	1	3 4 0	56.90
1.612	1	4 0 -2	57.10
1.597	1	1 1 4	57.68
1.583	1	4 2 1	58.22
1.538	2	4 0 2	60.12
1.524	1	1 2 4	60.72
1.452	3	4 2 2	64.06
1.448	2	2 5 -2	64.26
1.415	1	2 2 4	65.96
1.3327	1	1 6 -2	70.62
1.2913	1	3 5 2	73.24
1.2883	2	2 0 -5	73.44
1.2216	1	1 6 -3	78.18
1.2185	1	3 5 -3	78.42
1.1708	1	1 7 -2	82.28

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.760	25	0 0 1	13.09
5.541	1	1 1 0	15.98
5.370	5	0 1 1	16.49
4.421	1	0 2 0	20.07
4.382	20	1 1 -1	20.25
4.195	87	1 1 1	21.16
3.555	5	2 0 0	25.03
3.325	5	1 2 -1	26.79
3.299	9	2 1 0	27.01
3.241	9	1 2 1	27.50
3.223	9	2 0 -1	27.65
3.157	3	0 1 2	28.24
3.075	100	2 0 1	29.01
3.028	1	2 1 -1	29.47
2.944	1	1 1 -2	30.33
2.830	2	1 1 2	31.58
2.723	7	1 3 0	32.87
2.702	10	0 3 1	33.13
2.685	9	0 2 2	33.34
2.550	10	1 2 -2	35.16
2.545	2	1 3 -1	35.24
2.525	12	2 2 1	35.53
2.522	1	2 0 -2	35.56
2.426	7	2 1 -2	37.03
2.383	1	2 0 2	37.72
2.301	1	2 1 2	39.12
2.289	3	3 1 0	39.32
2.211	10	0 4 0	40.79
2.205	3	3 1 -1	40.88
2.191	12	2 2 -2	41.17

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.143	3	1 3 -2	42.13
2.128	3	2 3 1	42.44
2.111	2	1 4 0	42.80
2.025	2	3 2 -1	44.72
2.008	14	0 2 3	45.12
2.005	7	1 4 1	45.18
1.958	7	1 2 -3	46.33
1.916	1	2 3 -2	47.40
1.908	2	2 1 -3	47.62
1.907	2	1 2 3	47.65
1.849	11	3 1 2	49.24
1.847	1	3 3 0	49.30
1.818	1	3 2 -2	50.13
1.802	4	3 3 -1	50.61
1.795	5	2 4 1	50.83
1.790	1	0 3 3	50.97
1.778	1	4 0 0	51.36
1.777	1	1 4 2	51.38
1.762	1	3 3 1	51.85
1.718	2	1 3 3	53.29
1.716	2	1 5 0	53.34
1.711	2	4 1 -1	53.52
1.696	2	4 0 1	54.04
1.665	1	4 1 1	55.10
1.658	3	1 5 1	55.37
1.652	2	3 1 -3	55.59
1.652	1	3 3 -2	55.59
1.622	1	4 2 -1	56.70
1.617	1	3 4 0	56.91
1.612	1	4 0 -2	57.11
1.597	1	1 1 4	57.68
1.583	1	4 2 1	58.23
1.538	2	4 0 2	60.12
1.524	2	1 2 4	60.72
1.452	4	4 2 2	64.06
1.448	1	2 5 -2	64.29
1.415	1	2 2 4	65.95
1.3327	1	1 6 -2	70.62
1.3112	1	2 5 -3	71.95
1.2915	1	3 5 2	73.23
1.2883	1	2 0 -5	73.44
1.2216	2	1 6 -3	78.18
1.2186	1	3 5 -3	78.41
1.1787	1	6 0 -1	81.61
1.1709	1	1 7 -2	82.27
1.1267	1	0 0 6	86.26
1.0983	1	4 1 -5	89.07

Magnesium Phosphate, alpha, $Mg_2P_2O_7$

Structure

Monoclinic, $P2_1/c$ (14), [Calvo, 1967]. Z is assumed to be 4, not 2,as given by Calvo[1967].

Lattice parameters

a=6.891±.005, b=8.295±.005, c=9.072±.005Å, β=113.0±.1° [ibid.]

Density

(calculated) 3.18 g/cm³ [ibid.]

Thermal parameters

Isotropic:

Mg(1)	0.26
Mg(2)	0.33
P (1)	0.17
P (2)	0.13
O_I (1)	0.38
O_{II}(1)	0.32
O_{II}(2)	0.37
O_{III}(1c)	0.31
O_{III}(1t)	0.57
O_{III}(2c)	0.14
O_{III}(2t)	0.48

Atomic positions

The atomic parameters given by Calvo [1967] are for a related non-primitive space group setting $B2_1/c$. Those parameters were converted by a matrix to the corresponding values for $P2_1/c$,to facilitate computer calculations.

Polymorphism

A high-temperature polymorph, β-$Mg_2P_2O_7$, has the thortveitite structure. The transition occurs at 68 °C.with apparent coexistence of both α and β phases over an extended temperature interval.[ibid.]

Scattering factors

Mg^{+2}, P^{0}, O^{-1} [3.3.1A]

Scale factor

(integrated intensities) 2.543 × 10^4

Additional patterns

1. PDF card 8-38 [Menary, African Explosives and Chemical Industries Ltd., Transvaal, South Africa]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ*(°) λ = 1.54056 Å
6.42	1	1 0 0	13.78
5.09	3	-1 1 1	17.40
4.367	3	-1 0 2	20.32
4.149	16	0 2 0	21.40
3.864	1	-1 1 2	23.00
3.844	3	1 1 1	23.12
3.714	1	0 2 1	23.94
3.490	3	-1 2 1	25.50
3.213	4	2 0 0	27.74
3.007	100	-1 2 2 +	29.68
2.944	1	0 2 2	30.34
2.838	2	-1 1 3	31.50
2.671	1	-2 2 1	33.52
2.639	1	0 1 3	33.94
2.624	2	0 3 1	34.14
2.540	9	2 2 0 +	35.30
2.434	5	1 2 2	36.90
2.174	3	1 1 3	41.50
2.100	11	-2 3 2 +	43.04
2.074	2	3 1 0 +	43.60
2.040	1	-1 3 3	44.38
2.016	2	-3 2 2	44.92
2.012	1	0 4 1	45.02
1.873	3	-1 4 2	48.56
1.865	5	0 2 4 +	48.80
1.730	3	3 2 1	52.88
1.707	5	1 4 2 +	53.64
1.693	1	3 3 0	54.12
1.641	2	2 2 3 +	55.98
1.638	3	0 1 5	56.12
1.627	1	0 5 1 +	56.50
1.614	3	-4 0 4	57.02
1.607	3	1 5 0 +	57.30
1.574	7	-3 3 4	58.58
1.541	2	3 2 2 +	59.96
1.503	2	2 0 4 +	61.66
1.476	3	-4 3 2 +	62.92
1.471	3	0 4 4	63.14
1.413	2	2 2 4	66.08
1.383	2	0 6 0	67.72
1.358	1	-1 4 5	69.12
1.353	2	2 4 3	69.38
1.338	1	-5 1 4 +	70.28
1.335	2	-5 1 1 +	70.50
1.325	4	-2 3 6 +	71.06
1.322	2	2 3 4	71.28
1.318	1	4 1 2	71.54
1.270	1	5 1 0 +	74.68
1.256	2	1 6 2	75.66
1.217	1	2 4 4 +	78.54

Calculated Pattern *(Integrated)*					
d (Å)	*I*	*hkl*			2θ(°) λ = 1.54056 Å
6.43	3	1	0	0	13.77
5.09	6	-1	1	1	17.39
4.366	7	-1	0	2	20.32
4.175	4	0	0	2	21.26
4.147	35	0	2	0	21.41
3.864	1	-1	1	2	23.00
3.845	5	1	1	1	23.11
3.715	2	0	2	1	23.94
3.489	6	-1	2	1	25.51
3.213	10	2	0	0	27.74
3.008	72	-2	1	2	29.67
3.007	100	-1	2	2	29.69
3.006	86	1	0	2	29.70
2.998	1	1	2	1	29.78
2.996	4	2	1	0	29.80
2.943	1	0	2	2	30.35
2.838	4	-1	1	3	31.49
2.671	2	-2	2	1	33.53
2.639	3	0	1	3	33.94
2.625	4	0	3	1	34.13
2.542	3	-1	3	1	35.28
2.540	18	2	2	0	35.31
2.540	4	1	3	0	35.31
2.434	13	1	2	2	36.90
2.305	1	0	3	2	39.04
2.245	2	2	2	1	40.14
2.183	1	-1	1	4	41.33
2.174	8	1	1	3	41.49
2.100	22	-2	3	2	43.04
2.099	9	2	1	2	43.06
2.088	1	0	0	4	43.30
2.074	5	3	1	0	43.60
2.074	1	0	4	0	43.61
2.040	2	-1	3	3	44.38
2.016	4	-3	2	2	44.93
2.013	1	0	4	1	45.01
1.974	1	-1	4	1	45.93
1.920	1	2	3	1	47.29
1.873	6	-1	4	2	48.56
1.866	4	-3	1	4	48.76
1.865	16	0	2	4	48.80
1.791	1	1	0	4	50.96
1.751	1	-1	3	4	52.20
1.745	1	-4	0	2	52.38
1.730	7	3	2	1	52.88
1.710	1	-1	4	3	53.56
1.708	5	-4	1	2	53.62
1.707	6	1	4	2	53.65
1.707	4	2	3	2	53.65
1.698	1	-3	3	3	53.95
1.693	3	3	3	0	54.12
1.660	1	3	0	2	55.29
1.648	1	-1	2	5	55.72
1.642	2	-2	4	3	55.97
1.641	3	2	2	3	56.00
1.637	5	0	1	5	56.13
1.628	2	3	1	2	56.47
1.627	3	0	5	1	56.51
1.614	9	-4	0	4	57.01
1.607	2	4	0	0	57.30
1.606	5	1	5	0	57.31
1.574	22	-3	3	4	58.58
1.550	2	-3	2	5	59.59
1.542	1	-3	4	2	59.93
1.542	1	0	5	2	59.95
1.542	4	3	2	2	59.96
1.504	1	-2	4	4	61.63
1.503	4	2	0	4	61.67
1.476	6	-4	3	2	62.92
1.476	2	-2	5	2	62.94
1.471	7	0	4	4	63.14
1.452	2	4	1	1	64.10
1.413	5	2	2	4	66.07
1.402	1	3	4	1	66.64
1.395	1	1	2	5	67.02
1.391	1	-5	0	2	67.27
1.383	6	0	6	0	67.72
1.364	1	0	6	1	68.77
1.358	2	-1	4	5	69.13
1.354	5	2	4	3	69.37
1.339	3	-5	1	4	70.26
1.338	2	-1	5	4	70.31
1.336	2	1	5	3	70.42
1.335	3	-5	1	1	70.51
1.326	4	-4	1	6	71.03
1.326	9	-2	3	6	71.06
1.320	1	2	3	4	71.38
1.319	1	0	2	6	71.43
1.318	1	4	1	2	71.54
1.312	2	3	5	0	71.93
1.270	3	5	1	0	74.67
1.270	1	2	6	0	74.68
1.262	1	1	0	6	75.23
1.256	6	1	6	2	75.65
1.251	1	-1	1	7	76.04
1.238	2	0	6	3	76.94
1.237	2	-2	2	7	77.04
1.218	2	-5	3	4	78.48
1.217	2	2	4	4	78.54
1.208	1	-5	0	6	79.20

Reference

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

Manganese Vanadium Oxide, $Mn_2V_2O_7$

Structure
Monoclinic, C2/m (12), Z=2. The structure was determined by Dorm and Marinder [1967].

Lattice parameters
a=6.710±.002,b=8.726±.002,c=4.970±.001Å, β=103.57±.01° [ibid.]

Density
(calculated) 3.801 g/cm³

Thermal parameters
Isotropic [ibid.]

Scattering factors
Mn^0, V^0, O^{-1} [3.3.1A]

Scale factor
(integrated intensities) 2.738 x 10^4

Additional patterns
1. Brisi [1958]

Reference

Brisi, C. (1958). Ann. Chim. (Rome)48,270.
Dorm, E. and B. Marinder (1967). Acta Chem. Scand. 21, 590.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.224	17	1 1 0	16.96
4.828	1	0 0 1	18.36
4.362	6	0 2 0	20.34
3.935	2	-1 1 1	22.58
3.255	53	1 1 1 +	27.38
3.238	100	0 2 1	27.52
3.056	49	-2 0 1	29.20
2.656	11	1 3 0	33.72
2.612	19	2 2 0	34.30
2.449	6	2 0 1	36.66
2.428	4	-1 3 1	37.00
2.416	3	0 0 2	37.18
2.368	5	-1 1 2	37.96
2.239	9	1 3 1	40.24
2.205	4	-2 0 2	40.90
2.181	4	0 4 0	41.36
2.136	1	2 2 1	42.28
2.119	15	-3 1 1	42.64
2.112	10	3 1 0 +	42.78
2.051	2	1 1 2	44.12
1.999	6	0 4 1	45.58
1.967	13	-2 2 2	46.10
1.806	1	-3 1 2	50.50
1.790	2	3 1 1	50.98
1.776	4	-2 4 1	51.42
1.754	4	2 0 2	52.10
1.747	3	-3 3 1	52.34
1.742	5	3 3 0	52.50
1.708	18	1 3 2	53.62
1.686	3	1 5 0	54.38
1.631	8	4 0 0 +	56.38
1.627	6	2 2 2	56.52
1.623	3	-1 5 1	56.66
1.619	1	0 4 2	56.82
1.610	1	0 0 3	57.16
1.601	1	-2 0 3	57.52
1.562	7	1 5 1	59.08
1.559	16	-3 3 2 +	59.24
1.550	3	-2 4 2	59.58
1.548	5	3 3 1	59.68
1.528	2	-4 0 2	60.54
1.503	2	-2 2 3	61.66
1.4634	3	1 1 3	63.52
1.4544	5	0 6 0	63.96
1.4503	3	-3 1 3	64.16
1.4395	8	-1 3 3	64.70
1.4356	6	3 1 2	64.90
1.4235	3	-1 5 2	65.52
1.3722	3	4 2 1	68.30
1.3634	4	-3 5 1	68.80

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.3606	3	3 5 0	68.96
1.3255	1	2 0 3 +	71.06
1.3133	3	-2 6 1	71.82
1.2685	2	2 2 3	74.78
1.2668	2	-5 1 2	74.90
1.2545	1	-4 2 3	75.76
1.2514	2	-4 4 2 +	75.98
1.2306	1	-2 0 4	77.50
1.2285	2	-1 1 4	77.66
1.2250	1	4 0 2	77.92
1.1996	1	-1 7 1	79.90
1.1902	1	5 3 0	80.66
1.1800	1	5 1 1	81.50
1.1641	1	0 2 4	82.86
1.1307	3	1 5 3	85.88
1.1240	2	-3 5 3	86.52
1.1178	3	3 5 2 +	87.12
1.0934	1	-3 3 4	89.58
1.0852	3	4 6 0 +	90.44
1.0733	4	-5 3 3 +	91.72
1.0719	1	-2 4 4	91.88
1.0687	1	-4 2 4	92.24
1.0640	2	0 8 1 +	92.76
1.0614	1	1 3 4	93.06
1.0593	1	-6 2 2	93.30
1.0549	2	6 2 0 +	93.80
1.0536	1	-4 6 2	93.96
1.0344	2	2 8 0	96.26
1.0323	2	-5 5 2 +	96.52
1.0299	2	3 7 1	96.82
1.0113	2	-1 5 4	99.22
.9873	2	5 3 2	102.56
.9838	2	5 5 1	103.06
.9776	1	-2 8 2	103.98
.9673	1	-2 2 5	105.56
.9663	1	0 0 5 +	105.72
.9371	1	-1 3 5	110.56
.9328	1	-4 0 5	111.34
.9263	1	2 8 2 +	112.52
.9129	2	-4 8 1	115.08
.9096	1	-7 3 1 +	115.74
.9013	1	-2 8 3 +	117.44
.8989	1	-7 1 3	117.94

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.224	15	1 1 0	16.96
4.831	1	0 0 1	18.35
4.363	6	0 2 0	20.34
3.935	2	-1 1 1	22.58
3.261	1	2 0 0	27.32
3.255	49	1 1 1	27.38
3.238	100	0 2 1	27.52
3.056	52	-2 0 1	29.20
2.657	12	1 3 0	33.71
2.612	21	2 2 0	34.30
2.450	7	2 0 1	36.65
2.428	4	-1 3 1	37.00
2.416	3	0 0 2	37.19
2.369	6	-1 1 2	37.95
2.239	10	1 3 1	40.24
2.204	6	-2 0 2	40.91
2.181	5	0 4 0	41.35
2.136	1	2 2 1	42.28
2.118	18	-3 1 1	42.65
2.113	1	0 2 2	42.75
2.110	3	3 1 0	42.83
2.051	3	1 1 2	44.13
1.988	7	0 4 1	45.59
1.967	17	-2 2 2	46.10
1.806	1	-3 1 2	50.50
1.790	3	3 1 1	50.98
1.776	5	-2 4 1	51.42
1.754	5	2 0 2	52.09
1.746	3	-3 3 1	52.35
1.741	5	3 3 0	52.50
1.708	25	1 3 2	53.62
1.686	4	1 5 0	54.37
1.631	10	4 0 0	56.38
1.629	1	2 4 1	56.43
1.628	3	2 2 2	56.49
1.623	1	-1 5 1	56.68
1.619	1	0 4 2	56.82
1.610	2	0 0 3	57.15
1.601	2	-2 0 3	57.53
1.563	9	1 5 1	59.07
1.558	12	-3 3 2	59.24
1.558	7	-4 2 1	59.25
1.551	2	-2 4 2	59.58
1.548	6	3 3 1	59.68
1.528	3	-4 0 2	60.54
1.503	4	-2 2 3	61.67
1.4635	5	1 1 3	63.52
1.4543	7	0 6 0	63.96
1.4491	2	-3 1 3	64.22
1.4395	11	-1 3 3	64.70

Manganese Vanadium Oxide, $Mn_2V_2O_7$ – continued

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.4353	3	3 1 2	64.91
1.4236	5	-1 5 2	65.51
1.3723	5	4 2 1	68.29
1.3633	6	-3 5 1	68.81
1.3610	3	3 5 0	68.94
1.3258	1	2 0 3	71.04
1.3251	1	-4 4 1	71.08
1.3132	5	-2 6 1	71.83
1.2685	2	2 2 3	74.78
1.2667	2	-5 1 2	74.90
1.2544	2	-4 2 3	75.77
1.2515	2	-4 4 2	75.97
1.2506	1	2 6 1	76.04
1.2306	2	-2 0 4	77.50
1.2285	3	-1 1 4	77.66
1.2248	1	4 0 2	77.94
1.2051	1	4 4 1	79.46
1.1995	2	-1 7 1	79.90
1.1903	3	5 3 0	80.65
1.1801	3	5 1 1	81.49
1.1640	2	0 2 4	82.86
1.1308	4	1 5 3	85.88
1.1241	3	-3 5 3	86.51
1.1196	1	2 6 2	86.94
1.1183	2	-6 0 1	87.07
1.1176	4	3 5 2	87.14
1.0933	2	-3 3 4	89.58
1.0854	3	4 6 0	90.42
1.0851	3	3 3 3	90.45
1.0733	6	-5 3 3	91.72
1.0732	2	1 7 2	91.73
1.0718	1	-2 4 4	91.89
1.0685	2	-4 2 4	92.25
1.0640	4	0 8 1	92.77
1.0634	1	-5 5 1	92.83
1.0619	1	1 3 4	93.00
1.0592	2	-6 2 2	93.31
1.0549	1	2 0 4	93.81
1.0549	2	6 2 0	93.81
1.0535	1	-4 6 2	93.97
1.0344	3	2 8 0	96.26
1.0330	1	-3 7 2	96.43
1.0323	3	-5 5 2	96.52
1.0300	2	3 7 1	96.81
1.0113	3	-1 5 4	99.22
1.0059	1	-5 1 4	99.96
.9961	1	-1 7 3	101.31
.9872	4	5 3 2	102.57
.9838	3	5 5 1	103.07
.9776	2	-2 8 2	103.98

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
.9673	2	-2 2 5	105.56
.9663	2	0 0 5	105.72
.9657	1	-3 1 5	105.82
.9394	1	-2 6 4	110.16
.9373	1	-1 3 5	110.54
.9328	2	-4 0 5	111.34
.9265	1	7 1 0	112.47
.9263	1	2 8 2	112.52
.9152	1	3 3 4	114.63
.9143	1	6 0 2	114.80
.9129	3	-4 8 1	115.08
.9096	2	-7 3 1	115.73
.9092	1	5 1 3	115.82
.9014	2	-2 8 3	117.42
.9013	1	5 7 0	117.45
.9006	1	-7 3 2	117.58
.8989	1	-7 1 3	117.95

Methanesulfonanilide, $C_6H_5-NH-SO_2CH_3$

Structure
Monoclinic, $P2_1/c$ (14), Z=4 [Klug,1968]

Lattice parameters
a=9.203±.007,b=8.217±.005,c=11.026±.006Å
β=103.71°±.06° [ibid.]

Density
(calculated) 1.41 g/cm³ [ibid.]

Thermal parameters
Isotropic: H(12) through H(20) [ibid.]

S(1)	3.00
O(2)	4.17
O(3)	4.38
N(4)	3.29
C(5)	4.58
C(6)	2.93
C(7)	3.98
C(8)	4.48
C(9)	4.52
C(10)	4.66
C(11)	3.91

Scattering factors
N^0, O^0 [3.3.1A]
C^0 [Berghuis et al.,1955]
S^0 [Dawson, 1960]
H^0 [Stewart et al., 1965]

Scale factor
(Integrated intensities) 2.385×10^4

Reference

Berghuis, J., IJ. M. Haanapel, M. Potters, B.O. Loopstra, C.H. MacGillavry, and A. L. Veenendaal (1955). Acta Cryst. 8,478.
Dawson, B. (1960). Acta Cryst. 13, 403.
Klug, H.P. (1968). Acta Cryst. B24, 792.
Stewart, R.F., E.R.Davidson, and W.T.Simpson (1965). J. Chem. Phys. 42, 3175.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
8.93	11	1	0	0		9.90
6.52	21	0	1	1		13.58
6.05	52	1	1	0		14.64
5.67	4	-1	1	1		15.62
5.36	100	0	0	2		16.54
5.163	45	-1	0	2		17.16
4.940	5	1	1	1		17.94
4.485	26	0	1	2		19.78
4.471	29	2	0	0		19.84
4.371	99	-1	1	2		20.30
4.180	22	1	0	2		21.24
4.107	48	0	2	0		21.62
3.928	55	2	1	0	+	22.62
3.834	9	0	2	1		23.18
3.732	22	1	2	0	+	23.82
3.639	17	-1	2	1		24.44
3.537	5	-2	1	2		25.16
3.422	5	1	2	1		26.02
3.317	15	-1	1	3		26.86
3.259	30	0	2	2		27.34
3.042	8	-2	2	1		29.34
3.025	9	2	2	0		29.50
2.966	1	-2	1	3		30.10
2.893	2	2	1	2		30.88
2.879	1	1	1	3		31.04
2.872	2	-3	1	1		31.12
2.836	34	-2	2	2		31.52
2.801	10	3	1	0		31.92
2.796	12	2	2	1		31.98
2.746	1	-3	1	2		32.58
2.719	1	-1	2	3		32.92
2.677	9	0	0	4		33.44
2.654	1	0	3	1		33.74
2.608	16	-1	1	4		34.36
2.546	3	0	1	4		35.22
2.490	2	-3	1	3		36.04
2.464	7	-2	1	4	+	36.44
2.457	5	-3	2	1		36.54
2.420	2	-1	3	2		37.12
2.412	2	3	2	0		37.24
2.376	3	3	0	2		37.84
2.335	2	2	3	0		38.52
2.282	5	3	1	2	+	39.46
2.278	5	-3	0	4		39.52
2.262	1	3	2	1		39.82
2.244	2	0	2	4	+	40.16
2.235	4	4	0	0		40.32
2.195	2	-3	1	4		41.08
2.185	2	-1	3	3		41.28
2.180	2	-4	1	2		41.38

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.145	1	2 2 3	42.10
2.042	1	-3 3 1	44.32
2.025	1	2 1 4	44.72
2.017	3	3 3 0 +	44.90
1.996	2	-3 3 2	45.40
1.925	1	1 1 5	47.18
1.908	1	4 0 2	47.62
1.867	2	2 4 0	48.74
1.863	2	4 2 1	48.84
1.842	1	3 2 3	49.44
1.819	3	-2 4 2	50.10
1.809	1	2 4 1	50.40
1.792	4	-1 1 6	50.92
1.787	3	-1 4 3 +	51.06
1.770	2	-2 1 6	51.60
1.751	4	-3 3 4 +	52.18
1.745	2	-4 3 2	52.40
1.731	2	4 2 2 +	52.84
1.685	2	-3 1 6	54.40
1.640	1	5 2 0	56.04
1.608	1	-2 4 4	57.26
1.587	1	5 0 2	58.08
1.511	1	-2 3 6	61.28
1.458	1	-3 3 6	63.80
1.451	1	2 5 2	64.12
1.436	1	-6 2 2	64.90
1.432	1	-3 5 2	65.10
1.376	1	-4 3 6	68.10
1.373	1	3 1 6	68.24

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
8.94	9	1 0 0	9.88
6.52	19	0 1 1	13.57
6.05	47	1 1 0	14.63
5.67	4	-1 1 1	15.61
5.36	91	0 0 2	16.54
5.166	42	-1 0 2	17.15
4.940	5	1 1 1	17.94
4.487	21	0 1 2	19.77
4.470	18	2 0 0	19.84
4.373	100	-1 1 2	20.29
4.179	22	1 0 2	21.24
4.109	47	0 2 0	21.61
3.927	56	2 1 0	22.62
3.919	3	-2 0 2	22.67
3.836	9	0 2 1	23.17
3.733	21	1 2 0	23.81
3.725	5	1 1 2	23.87
3.639	18	-1 2 1	24.44
3.537	5	-2 1 2	25.15
3.422	5	1 2 1	26.02
3.317	15	-1 1 3	26.86
3.260	32	0 2 2	27.34
3.042	8	-2 2 1	29.34
3.025	9	2 2 0	29.50
2.967	1	-2 1 3	30.09
2.893	2	2 1 2	30.89
2.880	1	1 1 3	31.03
2.872	2	-3 1 1	31.12
2.836	38	-2 2 2	31.52
2.802	9	3 1 0	31.92
2.796	8	2 2 1	31.98
2.747	1	-3 1 2	32.57
2.718	1	-1 2 3	32.92
2.678	10	0 0 4	33.43
2.654	1	0 3 1	33.75
2.609	19	-1 1 4	34.35
2.546	3	0 1 4	35.22
2.490	2	-3 1 3	36.04
2.464	7	-2 1 4	36.43
2.462	1	1 2 3	36.47
2.457	1	-3 2 1	36.55
2.420	2	-1 3 2	37.12
2.412	1	3 2 0	37.24
2.376	4	3 0 2	37.83
2.335	2	2 3 0	38.52
2.286	2	-1 2 4	39.39
2.282	4	3 1 2	39.45
2.278	3	-3 0 4	39.52
2.262	1	3 2 1	39.81
2.245	1	-2 3 2	40.13

Methanesulfonanilide, C_6H_5–NH–SO_2CH_3 – continued

d (Å)	I	hkl	$2\theta(°)$ λ = 1.54056 Å
2.243	2	0 2 4	40.16
2.235	4	4 0 0	40.32
2.196	2	-3 1 4	41.08
2.185	2	-1 3 3	41.28
2.181	1	-4 1 2	41.36
2.145	2	2 2 3	42.10
2.042	1	-3 3 1	44.32
2.025	1	2 1 4	44.72
2.017	1	0 4 1	44.89
2.017	3	3 3 0	44.91
1.996	2	-3 3 2	45.40
1.963	1	4 2 0	46.20
1.941	1	-1 3 4	46.76
1.925	1	1 1 5	47.18
1.908	1	4 0 2	47.61
1.867	2	2 4 0	48.74
1.864	1	4 2 1	48.83
1.842	1	3 2 3	49.45
1.819	3	-2 4 2	50.09
1.809	1	2 4 1	50.41
1.792	4	-1 1 6	50.91
1.787	1	-1 4 3	51.06
1.785	1	0 0 6	51.12
1.770	2	-2 1 6	51.59
1.752	5	-3 3 4	52.18
1.751	1	3 1 4	52.20
1.744	2	-4 3 2	52.42
1.732	1	4 3 0	52.82
1.731	1	4 2 2	52.86
1.685	2	-3 1 6	54.39
1.640	1	5 2 0	56.04
1.608	2	-2 4 4	57.25
1.587	1	5 0 2	58.08
1.542	1	2 5 0	59.92
1.512	1	-2 3 6	61.27
1.458	2	-3 3 6	63.79
1.451	1	2 5 2	64.13
1.439	1	3 5 0	64.72
1.436	1	-6 2 2	64.89
1.431	1	-3 5 2	65.11
1.376	1	-4 3 6	68.10
1.373	1	3 1 6	68.24

Structure

Hexagonal, R32 (155) or $R\bar{3}m$ (166), Z = 3 (hexagonal cell) [Pauling, 1929]. The structure was refined and the space group determined as $R\bar{3}m$ by Ferrari et al., [1963].

Lattice parameters

a= 3.478 ±.001, c= 17.41 ±.12 [Ferrari et al., 1963].

Density

(calculated) 3.540 g/cm^3

Thermal parameters

Isotropic, overall B = 2.0

Scattering factors

Cl^0 [3.3.1A]
Ni^0 [3.3.1B]

Scale factor

(integrated intensities) 1.668×10^4

Additional patterns

1. PDF card 1-1134[Hanawalt et al.,1938]

Reference

Ferrari, A., A. Braibanti and G. Bigliardi (1963). Acta Cryst. **16**, 846.

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

Pauling, L. (1929). Proc.Natl. Acad.Sci.US 15, 709.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.80	100	0 0 3	15.26
2.97	30	1 0 1	30.08
2.48	79	1 0 4	36.24
2.28	8	0 1 5	39.52
1.93	1	0 0 9	46.94
1.92	10	1 0 7	47.36
1.76	18	0 1 8	51.78
1.74	17	1 1 0	52.58
1.67	8	1 1 3	55.08
1.50	2	0 2 1	61.78
1.45	2	0 0 12	64.14
1.42	6	0 2 4	65.54
1.40	3	0 1 11	66.70
1.38	1	2 0 5	67.74
1.29	1	1 1 9	73.12
1.29	1	0 2 7	73.44
1.24	3	2 0 8	76.92
1.14	1	2 1 1	85.38
1.11	3	1 1 12	87.48
1.10	3	2 1 4	88.76
1.09	1	2 0 11	89.82
1.04	1	2 1 7	96.16
1.02	1	1 0 16	97.64
1.01	2	1 2 8	99.56
1.00	1	3 0 0	100.20
.965	1	1 1 15	105.86
.826	1	3 0 12 +	137.82
.820	1	1 3 4	139.74
.787	1	2 1 16	156.62

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.80	93	0 0 3	15.25
2.97	37	1 0 1	30.08
2.85	1	0 1 2	31.40
2.48	100	1 0 4	36.24
2.28	11	0 1 5	39.53
1.93	2	0 0 9	46.93
1.92	14	1 0 7	47.36
1.76	27	0 1 8	51.78
1.74	26	1 1 0	52.58
1.67	12	1 1 3	55.08
1.50	3	0 2 1	61.78
1.45	4	0 0 12	64.14
1.42	11	0 2 4	65.53
1.40	4	0 1 11	66.70
1.38	2	2 0 5	67.73
1.29	2	1 1 9	73.11
1.29	2	0 2 7	73.44
1.24	6	2 0 8	76.92
1.16	1	0 0 15	83.16
1.14	2	2 1 1	85.38
1.11	7	1 1 12	87.49
1.10	7	2 1 4	88.75
1.09	1	2 0 11	89.82
1.08	1	1 2 5	90.77
1.04	2	2 1 7	96.17
1.02	2	1 0 16	97.65
1.01	5	1 2 8	99.56
1.00	3	3 0 0	100.21
.965	2	1 1 15	105.86
.924	2	1 2 11	112.91
.882	2	0 2 16	121.70
.877	1	1 0 19	122.96
.870	2	2 2 0	124.72
.860	1	2 2 3	127.22
.836	2	0 1 20	134.17
.834	1	1 3 1	134.77
.826	2	0 3 12	137.81
.826	2	3 0 12	137.81
.820	5	1 3 4	139.73
.812	1	3 1 5	142.97
.792	2	1 3 7	153.15
.787	6	2 1 16	156.61
.783	2	0 2 19	159.47

Nickel Phosphide, $Ni_{12}P_5$

Structure

Tetragonal, I4/m (87), Z=2 [Rundqvist and Larsson, 1959]

Lattice parameters

a=8.646, c=5.070Å [ibid.]

Density

(calculated) 7.53 g/cm^3 [ibid]

Thermal parameters

Overall temperature factor, 0.49 [ibid.]

Scattering factors

Ni° [Thomas and Umeda, 1957]
P° [Tomiie and Stam, 1958]

Scale factor

[integrated intensities] 13.389 × 10^4

Reference

Rundqvist, S. and E. Larsson (1959). Acta Chem. Scan. **13**, 551.

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

Tomiie, Y. and C.H.Stam (1958). Acta Cryst. **11**, 126.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
4.37	4	0 1 1	20.30
4.32	3	0 2 0	20.54
3.07	3	2 1 1 +	29.02
3.056	3	2 2 0	29.20
2.735	16	3 1 0	32.72
2.535	2	0 0 2	35.38
2.505	9	0 3 1	35.82
2.341	42	1 1 2	38.42
2.186	18	0 2 2	41.26
2.167	22	2 3 1 +	41.64
2.162	33	0 4 0	41.74
2.038	20	3 3 0	44.42
1.933	65	2 4 0 +	46.96
1.859	100	3 1 2	48.96
1.696	7	5 1 0	54.04
1.645	3	0 4 2	55.86
1.636	8	0 5 1 +	56.16
1.588	3	3 3 2	58.02
1.537	7	2 4 2 +	60.14
1.531	2	2 5 1	60.42
1.458	1	0 3 3	63.80
1.409	2	5 1 2 +	66.26
1.381	3	2 3 3	67.78
1.367	4	6 2 0	68.60
1.316	1	1 4 3	71.66
1.305	1	5 4 1	72.36
1.280	3	3 5 2 +	74.00
1.268	7	0 0 4	74.84
1.253	1	0 6 2	75.88
1.249	1	3 6 1	76.14
1.223	6	7 1 0 +	78.10
1.209	2	0 5 3 +	79.18
1.203	11	2 6 2 +	79.60
1.200	7	6 4 0 +	79.88
1.150	1	3 1 4	84.12
1.135	2	3 7 0	85.46
1.101	10	5 5 2 +	88.76
1.093	3	0 4 4	89.58
1.084	4	6 4 2	90.58
1.081	4	6 5 1 +	90.84
1.076	3	3 3 4	91.40
1.060	10	2 4 4 +	93.22
1.049	4	8 1 1 +	94.48
1.015	2	5 1 4	98.70
1.005	1	5 7 0	100.06
.969	3	2 8 2	105.32
.967	3	4 8 0 +	105.68
.955	1	1 9 0	107.56
.934	2	5 7 2 +	111.08
.929	2	6 2 4	111.94

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
.926	1	6 5 3	112.56
.922	1	7 6 1	113.30
.911	1	9 3 0	115.38
.905	3	8 1 3 +	116.58
.880	4	7 1 4 +	122.16
.875	1	0 5 5	123.44
.871	2	6 4 4	124.34
.865	1	4 9 1 +	125.96
.846	2	3 7 4	131.24
.840	1	9 5 0 +	133.06
.837	1	1 1 6	133.92
.820	1	7 6 3 +	139.90
.818	3	6 8 2 +	140.54
.807	6	3 1 6	145.16
.805	4	5 8 3	146.08
.804	7	10 2 2 +	146.68
.803	1	4 10 0	147.32
.797	4	9 5 2 +	150.16
.790	1	6 9 1 +	154.62
.788	2	5 7 4	155.96
.783	3	1 11 0	159.50

Calculated Pattern (integrated)			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
4.37	3	0 1 1	20.29
4.32	2	0 2 0	20.53
3.07	2	2 1 1	29.02
3.075	1	1 2 1	29.02
3.057	2	2 2 0	29.19
2.734	14	3 1 0	32.73
2.535	1	0 0 2	35.38
2.505	8	0 3 1	35.81
2.342	40	1 1 2	38.41
2.187	17	0 2 2	41.25
2.168	2	3 2 1	41.63
2.168	16	2 3 1	41.63
2.162	23	0 4 0	41.75
2.038	19	3 3 0	44.42
1.938	7	1 4 1	46.85
1.933	16	4 2 0	46.96
1.933	43	2 4 0	46.96
1.859	100	3 1 2	48.96
1.696	7	5 1 0	54.04
1.645	4	0 4 2	55.85
1.637	3	4 3 1	56.15
1.637	2	3 4 1	56.15
1.637	3	0 5 1	56.15
1.588	3	3 3 2	58.02
1.537	1	4 2 2	60.14
1.537	6	2 4 2	60.14
1.531	1	2 5 1	60.43
1.458	2	0 3 3	63.79
1.409	2	5 1 2	66.26
1.409	1	1 5 2	66.26
1.381	3	2 3 3	67.78
1.367	5	6 2 0	68.59
1.316	2	1 4 3	71.66
1.305	1	5 4 1	72.36
1.280	2	5 3 2	74.00
1.280	8	3 5 2	74.00
1.267	9	0 0 4	74.85
1.253	1	0 6 2	75.89
1.249	1	3 6 1	76.14
1.223	4	7 1 0	78.10
1.223	1	5 5 0	78.10
1.223	2	1 7 0	78.10
1.209	1	4 3 3	79.18
1.209	1	3 4 3	79.18
1.209	1	0 5 3	79.18
1.203	6	6 2 2	79.61
1.203	9	2 6 2	79.61
1.200	1	0 7 1	79.86
1.199	3	6 4 0	79.95
1.150	1	3 1 4	84.11

Nickel Phosphide, $Ni_{12}P_5$ – continued

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.135	3	3 7 0	85.45
1.101	6	5 5 2	88.76
1.101	3	7 1 2	88.76
1.101	5	1 7 2	88.76
1.093	4	0 4 4	89.58
1.084	5	6 4 2	90.58
1.082	2	6 5 1	90.83
1.082	1	5 6 1	90.83
1.076	4	3 3 4	91.40
1.060	4	4 2 4	93.22
1.060	11	2 4 4	93.22
1.049	2	7 4 1	94.47
1.049	3	8 1 1	94.47
1.049	1	1 8 1	94.47
1.015	3	5 1 4	98.71
1.005	2	5 7 0	100.06
.997	1	0 7 3	101.15
.969	4	2 8 2	105.31
.967	1	8 4 0	105.66
.967	3	4 8 0	105.66
.955	1	1 9 0	107.56
.934	2	5 7 2	111.06
.934	1	2 3 5	111.13
.929	3	6 2 4	111.94
.926	1	6 5 3	112.57
.922	1	7 6 1	113.30
.911	2	9 3 0	115.38
.905	3	8 1 3	116.57
.905	1	1 8 3	116.57
.905	2	7 4 3	116.57
.894	1	9 1 2	119.10
.880	2	1 7 4	122.16
.880	5	7 1 4	122.16
.880	2	5 5 4	122.16
.875	1	0 5 5	123.43
.871	3	6 4 4	124.34
.865	2	4 9 1	125.87
.865	1	8 6 0	125.98
.848	1	10 2 0	130.61
.846	4	3 7 4	131.25
.840	2	9 5 0	133.05
.840	1	5 9 0	133.05
.837	3	1 1 6	133.92
.829	1	0 2 6	136.50
.826	1	7 7 2	137.76
.820	1	2 9 3	139.89
.820	1	7 6 3	139.89
.818	1	8 6 2	140.54
.818	5	6 8 2	140.54
.818	2	0 10 2	140.54

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
.808	2	2 8 4	144.89
.807	13	3 1 6	145.15
.806	1	5 8 3	145.92
.804	14	10 2 2	146.68
.804	8	2 10 2	146.68
.803	1	4 10 0	147.29
.797	1	5 9 2	150.15
.797	11	9 5 2	150.15
.797	1	3 6 5	150.29
.794	2	6 6 4	151.84
.790	2	6 9 1	154.62
.790	1	9 6 1	154.62
.788	7	5 7 4	155.97
.787	1	0 4 6	156.34
.784	2	0 7 5	158.74
.783	12	1 11 0	159.50

Structure

Orthorhombic, Fdd2 (43), Z=8. The structure was determined by de Decker [1941].

Lattice parameters

a = 16.3, b = 8.14, c = 5.26 Å [ibid.]

Density

(calculated) 2.70 g/cm^3 [ibid.]

Thermal parameters

Isotropic, overall B = 2.0

Polymorphism

de Decker and MacGillavry [1941] described a metastable rhombohedral form having the space group R3c (161). Hill, Faust, and Hendricks [1943] identified a third phase which was thought to be tetragonal but was later shown to be a different orthorhombic phase with space group Pnam (62) [MacGillavry et al., 1949].

Scattering factors

O°, P° [3.3.1A]

Scale factor

(integrated intensities) 11.79 x 10^4

Additional patterns

1. PDF card 5-318 [Hill et al.,1943].(incorrectly labelled "at 562 °C").
2. Thilo and Wieker [1954].

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(^\circ)$ λ = 1.54056 Å
4.26	100	1	1	1		20.82
4.07	3	4	0	0		21.80
3.64	5	2	2	0		24.42
3.43	14	3	1	1		25.98
2.88	41	4	2	0		31.04
2.62	20	5	1	1		34.16
2.39	7	1	3	1		37.68
2.21	3	0	2	2		40.82
2.06	1	7	1	1		43.92
2.04	2	0	4	0	+	44.48
1.939	8	5	3	1	+	46.82
1.889	2	6	0	2		48.12
1.821	2	8	2	0	+	50.04
1.705	1	1	1	3		53.72
1.675	3	9	1	1		54.74
1.517	3	5	1	3		61.02
1.497	5	4	4	2	+	61.94
1.448	3	9	3	1		64.26
1.440	1	8	4	0		64.68
1.404	2	5	5	1		66.56
1.315	1	0	0	4		71.72
1.312	2	10	2	2		71.92
1.263	1	8	4	2		75.18
1.206	2	0	6	2	+	79.40
1.196	1	4	2	4		80.18
1.143	1	9	3	3		84.78

Calculated Pattern *(Integrated)*					
d (Å)	I	hkl			$2\theta(°)$ $\lambda = 1.54056$ Å
4.26	100	1	1	1	20.81
4.07	9	4	0	0	21.79
3.64	6	2	2	0	24.43
3.43	15	3	1	1	25.97
2.88	43	4	2	0	31.03
2.62	24	5	1	1	34.15
2.39	8	1	3	1	37.68
2.21	9	0	2	2	40.82
2.06	1	7	1	1	43.92
2.04	1	8	0	0	44.43
2.03	2	0	4	0	44.48
1.942	4	4	2	2	46.74
1.939	9	5	3	1	46.82
1.890	2	6	0	2	48.11
1.822	2	8	2	0	50.02
1.821	1	4	4	0	50.06
1.705	1	1	1	3	53.73
1.676	4	9	1	1	54.73
1.548	1	1	5	1	59.67
1.517	4	5	1	3	61.03
1.498	1	8	2	2	61.90
1.497	7	4	4	2	61.94
1.448	4	9	3	1	64.27
1.440	1	8	4	0	64.68
1.421	1	3	3	3	65.63
1.404	3	5	5	1	66.56
1.342	1	5	3	3	70.05
1.315	1	0	0	4	71.71
1.312	2	10	2	2	71.93
1.272	1	10	4	0	74.53
1.263	1	8	4	2	75.16
1.206	1	13	1	1	79.37
1.206	3	0	6	2	79.41
1.196	2	4	2	4	80.17
1.190	1	1	5	3	80.69
1.180	1	9	5	1	81.51
1.143	2	9	3	3	84.78
1.120	1	5	5	3	86.87
.924	1	4	8	2	112.91

Reference

de Decker, H.C.J. (1941). Rec. Trav. Chim. 60, 413.

de Decker, H. C. J. and C. H. MacGillavry (1941). Rec. Trav. Chim. 60, 153.

Hill, W.L., G.T. Faust, and S.B. Hendricks (1943). J. Am. Chem. Soc. 65, 794.

MacGillavry, C.H., H.C.J. de Decker, and L.M. Nijland (1949). Nature 164, 448.

Thilo, E. and W. Wieker (1954). Z. anorg. u. allgem. Chem. 277, 27.

Structure

Orthorhombic, Pnam (62), Z=4. The structure was determined by MacGillavry et al. [1949]. Using their data, Cruickshank [1964] performed a least squares structure refinement.

Lattice parameters

a= 9.23, b= 7.18, c= 4.94Å [ibid.]

Density

(calculated) 2.880 g/cm^3

Thermal parameters

Isotropic, overall B=.55 [Cruickshank, 1964].

Atomic positions

Cruickshank [1964]

Polymorphism

Two other forms are known. One is metastable and has the rhombohedral space group R3c(161)[de Decker and MacGillavry 1941]. The other is a different stable orthorhombic phase with space group Fdd2 (43) [de Decker, 1941].

Scattering factors

O°, P° [3.3.1A]

Scale factor

(integrated intensities) 1.041 x 10^4

Additional patterns

1. PDF card 5-0488 [Hill et al., 1943]. (incorrectly labelled "at 580 °C")
2. Thilo and Wieker [1954]

Reference

Cruickshank, D.W.J. (1964). Acta Cryst.17, 677.

de Decker, H.C.J. (1941). Rec. Trav. Chim. 60, 413.

de Decker, H. C. J. and C. H. MacGillavry (1941). Rec. Trav. Chim. 60, 153.

Hill, W.L., G.T. Faust, and S.B. Hendricks (1943). J. Am. Chem. Soc. 65, 794.

MacGillavry, C. H., H.C.J. de Decker, and L. M. Nijland (1949). Nature 164, 448.

Thilo, E. and W. Wieker (1954). Z. anorg. u. allgem. Chem. 277, 27.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(^\circ)$ λ = 1.54056 Å
5.67	55	1	1	0		15.62
4.61	41	2	0	0		19.22
4.07	4	0	1	1		21.82
3.88	81	2	1	0		22.90
3.72	46	1	1	1		23.88
3.59	53	0	2	0		24.78
3.37	46	2	0	1		26.40
3.05	100	2	1	1		29.24
2.83	7	2	2	0	+	31.54
2.77	75	1	2	1		32.28
2.47	35	0	0	2		36.34
2.45	15	3	1	1	+	36.58
2.34	9	3	2	0		38.50
2.31	3	4	0	0		39.00
2.26	13	1	1	2		39.78
2.18	3	2	0	2		41.42
2.15	11	0	3	1		41.90
2.12	8	2	3	0		42.52
2.11	4	3	2	1		42.78
2.10	2	1	3	1		43.10
2.08	6	2	1	2		43.38
2.01	12	4	1	1		45.14
1.987	3	1	2	2		45.62
1.941	4	4	2	0		46.76
1.889	4	3	3	0		48.12
1.862	1	2	2	2		48.88
1.806	5	4	2	1		50.48
1.762	1	1	4	0	+	51.84
1.697	10	3	2	2		53.98
1.690	4	1	3	2		54.24
1.686	4	4	0	2		54.36
1.681	2	5	1	1		54.54
1.673	5	2	4	0		54.84
1.660	1	1	4	1		55.30
1.642	3	5	2	0	+	55.96
1.611	1	2	3	2		57.14
1.584	2	2	4	1		58.18
1.581	3	1	1	3		58.32
1.574	2	4	3	1		58.58
1.558	3	5	2	1		59.26
1.550	7	3	4	0	+	59.58
1.538	2	6	0	0		60.10
1.526	2	4	2	2		60.62
1.516	7	2	1	3		61.08
1.504	1	6	1	0		61.60
1.478	6	1	2	3	+	62.84
1.469	2	6	0	1		63.26
1.462	2	5	3	0		63.60
1.452	1	0	4	2		64.08
1.423	1	3	1	3		65.54

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.419	1	1 5 0	65.76
1.417	1	4 4 0	65.86
1.402	1	5 3 1	66.68
1.385	3	2 4 2	67.58
1.367	5	5 2 2	68.58
1.364	7	1 5 1	68.78
1.360	4	6 2 1	69.00
1.356	2	0 3 3	69.20
1.342	1	1 3 3	70.04
1.317	3	4 1 3	71.56
1.313	9	3 4 2	71.82
1.306	5	6 0 2	72.30
1.297	1	7 1 0	72.88
1.285	1	6 1 2	73.68
1.258	4	5 3 2 +	75.52
1.255	4	7 1 1 +	75.76
1.252	2	6 3 1	75.96
1.235	5	0 0 4	77.18
1.229	6	4 4 2	77.62
1.227	3	6 2 2	77.76
1.219	1	4 5 0	78.36
1.199	1	2 5 2	79.96
1.187	2	1 6 0	80.94
1.177	2	2 1 4	81.76
1.174	1	2 4 3	82.04
1.169	1	4 3 3	82.40
1.168	1	0 2 4	82.54
1.163	1	5 2 3	82.98
1.154	1	8 0 0	83.76
1.151	1	3 5 2	84.00
1.148	1	7 1 2	84.26
1.146	1	6 3 2	84.44
1.141	2	5 4 2	84.90
1.139	1	8 1 0	85.14
1.137	1	6 4 1	85.32
1.128	3	2 6 1 +	86.16
1.125	3	7 3 1 +	86.46
1.110	1	8 1 1	87.88
1.107	1	7 2 2	88.22
1.105	2	5 5 1	88.42
1.098	1	8 2 0	89.06
1.093	1	5 3 3 +	89.60
1.092	1	3 2 4	89.74
1.077	1	0 6 2	91.34
1.075	2	1 5 3	91.56
1.072	1	6 2 3	91.84
1.034	2	8 1 2	96.26
1.027	1	6 5 1	97.22
1.019	1	7 1 3	98.24
1.017	1	6 3 3	98.42

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.67	47	1 1 0	15.62
4.62	36	2 0 0	19.22
4.07	4	0 1 1	21.82
3.88	78	2 1 0	22.89
3.72	42	1 1 1	23.88
3.59	49	0 2 0	24.78
3.37	46	2 0 1	26.41
3.05	100	2 1 1	29.23
2.83	6	2 2 0	31.55
2.83	1	3 1 0	31.61
2.77	80	1 2 1	32.29
2.47	36	0 0 2	36.34
2.46	4	2 2 1	36.53
2.45	12	3 1 1	36.58
2.34	9	3 2 0	38.50
2.31	3	4 0 0	39.00
2.26	14	1 1 2	39.78
2.18	3	2 0 2	41.43
2.15	12	0 3 1	41.91
2.12	9	2 3 0	42.51
2.11	4	3 2 1	42.78
2.10	2	1 3 1	43.09
2.08	6	2 1 2	43.38
2.01	14	4 1 1	45.13
1.987	4	1 2 2	45.61
1.941	4	4 2 0	46.76
1.889	5	3 3 0	48.13
1.862	1	2 2 2	48.88
1.807	7	4 2 1	50.47
1.764	1	3 3 1	51.77
1.762	2	1 4 0	51.85
1.697	13	3 2 2	53.98
1.690	4	1 3 2	54.24
1.686	4	4 0 2	54.36
1.681	1	5 1 1	54.54
1.673	6	2 4 0	54.83
1.660	1	1 4 1	55.31
1.642	2	5 2 0	55.97
1.642	1	4 1 2	55.97
1.611	1	2 3 2	57.14
1.585	2	2 4 1	58.17
1.581	2	1 1 3	58.30
1.575	3	4 3 1	58.58
1.558	4	5 2 1	59.26
1.551	3	2 0 3	59.56
1.550	6	3 4 0	59.58
1.538	2	6 0 0	60.10
1.526	3	4 2 2	60.62
1.516	9	2 1 3	61.08
1.504	1	6 1 0	61.61

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.479	2	3 4 1	62.76
1.477	8	1 2 3	62.85
1.469	3	6 0 1	63.26
1.462	3	5 3 0	63.60
1.452	2	0 4 2	64.07
1.423	1	3 1 3	65.54
1.419	1	1 5 0	65.76
1.417	2	4 4 0	65.87
1.402	2	5 3 1	66.67
1.385	4	2 4 2	67.57
1.367	6	5 2 2	68.58
1.364	7	1 5 1	68.78
1.359	2	6 2 1	69.03
1.357	2	0 3 3	69.19
1.342	1	1 3 3	70.05
1.318	4	4 1 3	71.55
1.313	13	3 4 2	71.83
1.306	6	6 0 2	72.30
1.297	1	7 1 0	72.88
1.285	1	6 1 2	73.68
1.258	1	3 5 1	75.49
1.258	5	5 3 2	75.52
1.256	2	4 2 3	75.68
1.254	2	7 1 1	75.77
1.252	2	6 3 1	75.95
1.235	8	0 0 4	77.17
1.229	8	4 4 2	77.62
1.227	3	6 2 2	77.76
1.219	1	4 5 0	78.37
1.199	2	2 5 2	79.96
1.193	1	2 0 4	80.43
1.187	3	1 6 0	80.94
1.177	2	2 1 4	81.76
1.174	1	2 4 3	82.05
1.169	1	4 3 3	82.40
1.168	2	0 2 4	82.54
1.163	1	5 2 3	82.99
1.154	1	8 0 0	83.77
1.151	1	3 5 2	83.99
1.148	1	7 1 2	84.26
1.146	2	6 3 2	84.44
1.141	3	5 4 2	84.90
1.139	1	8 1 0	85.09
1.137	2	6 4 1	85.32
1.129	1	3 4 3	86.06
1.128	4	2 6 1	86.16
1.125	3	7 3 1	86.46
1.124	1	6 0 3	86.51
1.110	2	8 1 1	87.89
1.107	1	7 2 2	88.23

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.105	3	5 5 1	88.41
1.098	2	8 2 0	89.06
1.093	1	4 5 2	89.59
1.093	1	5 3 3	89.60
1.092	2	3 2 4	89.74
1.077	2	0 6 2	91.33
1.075	3	1 5 3	91.55
1.073	1	6 2 3	91.79
1.068	1	2 3 4	92.34
1.034	4	8 1 2	96.26
1.027	2	6 5 1	97.21
1.021	1	3 5 3	97.96
1.019	1	7 1 3	98.23
1.017	1	6 3 3	98.41
1.016	1	3 6 2	98.54
.994	2	2 4 4	101.66
.987	1	5 2 4	102.61
.976	1	4 6 2	104.24
.966	3	3 4 4	105.76
.963	1	6 0 4	106.23
.957	2	2 1 5	107.12
.955	2	3 7 1	107.57
.953	1	7 5 1	107.86
.953	1	6 4 3	107.90
.948	2	1 2 5	108.76
.947	3	2 6 3	108.79
.946	2	7 3 3	109.11
.943	2	5 3 4	109.48
.937	1	8 1 3	110.62
.934	2	5 5 3	111.18
.931	1	4 4 4	111.67
.930	2	5 6 2	111.80
.913	1	0 3 5	115.01
.901	2	4 1 5	117.49
.900	3	10 1 1	117.68
.899	1	8 5 0	117.84
.894	1	7 1 4	118.92
.893	3	1 8 0	119.15
.890	1	9 4 0	119.77
.886	1	7 6 0	120.74
.885	1	6 5 3	120.97
.876	2	9 4 1	123.04
.868	1	4 5 4	125.19
.856	4	1 6 4	128.36
.847	1	5 2 5	130.99
.843	2	8 0 4	132.03
.840	2	1 8 2	132.97
.838	3	3 7 3	133.70
.837	1	8 1 4	133.83
.837	1	7 5 3	134.08

Phosphorus Oxide (metastable form), P_4O_{10} (rhombohedral)

Structure

Rhombohedral, R3c (161), Z=2. The structure was determined by de Decker and MacGillavry [1941]. Using their data, Cruickshank[1964] refined the structure.

Lattice parameters

a= 7.44Å, α= 87°, [de Decker and MacGillavry, 1941]. The corresponding hexagonal parameters are a= 10.25, c= 13.55Å, with Z= 6 .

Density

(calculated) 2.30 g/cm^3 [de Decker and MacGillavry, 1941].

Thermal parameters

Isotropic P(1) 2.13
P(2) 1.95
O(3) 4.74
O(4) 1.81
O(5) 1.99
O(6) 2.70

Atomic positions

Cruickshank [1964]

Polymorphism

de Decker [1941] described a stable orthorhombic phase of P_2O_5 with a space group Fdd2 (43). Hill, Faust, and Hendricks [1943] identified a third form which was thought to be tetragonal but was later shown to be another orthorhombic phase with space group Pnam (62) [MacGillavry et al., 1949].

Scattering factors

O°, P° [3.3.1A]

Scale factor

(integrated intensities) 3.590 x 10^4

Additional patterns

1. PDF card 1-213 [Hanawalt et al., 1938]
2. Hill, Faust, and Hendricks [1943]
3. Thilo and Wieker [1954]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.39	100	1 1 0	16.44
5.12	76	-1 1 0	17.30
3.71	3	2 0 0	23.96
3.39	10	2 1 0	26.28
3.26	20	-2 1 0	27.36
3.17	12	2 1 1	28.16
3.01	21	2 1 -1	29.68
2.959	2	-2 1 1	30.18
2.563	3	-2 2 0	34.98
2.423	7	-2 2 1	37.08
2.384	1	3 1 0	37.70
2.314	4	-3 1 0	38.88
2.259	9	2 2 2	39.88
2.229	5	3 1 -1	40.44
2.108	2	3 2 0 +	42.86
2.067	3	3 2 1	43.76
2.014	1	-3 2 0	44.98
1.992	2	3 2 -1	45.50
1.951	8	3 -2 1	46.52
1.780	1	3 2 -2	51.28
1.694	1	4 2 0	54.08
1.677	1	4 2 1	54.68
1.664	2	3 3 2 +	55.14
1.628	1	-4 2 0	56.46
1.522	1	4 3 0	60.82
1.512	1	4 3 1	61.24
1.479	3	-4 2 2	62.76
1.422	1	-4 3 1	65.62
1.347	1	-4 3 2	69.78
1.327	1	-5 2 1	70.94
1.302	1	5 3 0	72.52
1.298	2	5 3 1	72.78
1.246	1	-4 3 3	76.34
1.238	1	4 4 -2 +	76.98
1.176	1	-5 3 2	81.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	$2\theta(°)$ $\lambda = 1.54056$ Å
5.39	100	1 1 0	16.44
5.12	76	-1 1 0	17.29
3.71	4	2 0 0	23.95
3.39	11	2 1 0	26.28
3.26	23	-2 1 0	27.36
3.17	14	2 1 1	28.17
3.01	26	2 1 -1	29.69
2.959	2	-2 1 1	30.18
2.562	4	-2 2 0	34.99
2.422	8	-2 2 1	37.08
2.384	2	3 1 0	37.70
2.314	5	-3 1 0	38.89
2.259	11	2 2 2	39.88
2.229	6	3 1 -1	40.44
2.109	2	-2 2 2	42.85
2.108	2	3 2 0	42.86
2.067	3	3 2 1	43.76
2.014	2	-3 2 0	44.98
1.992	2	3 2 -1	45.51
1.950	11	3 -2 1	46.53
1.780	1	3 2 -2	51.28
1.694	1	4 2 0	54.08
1.677	1	4 2 1	54.69
1.665	1	-3 3 1	55.12
1.664	2	3 3 2	55.15
1.628	1	-4 2 0	56.46
1.598	1	4 -2 1	57.64
1.583	1	-4 2 1	58.22
1.522	2	4 3 0	60.81
1.512	2	4 3 1	61.24
1.479	4	-4 2 2	62.75
1.421	1	-4 3 1	65.63
1.403	1	5 2 0	66.59
1.396	1	5 2 1	67.00
1.347	1	-4 3 2	69.76
1.327	1	-5 2 1	70.94
1.302	2	5 3 0	72.52
1.298	3	5 3 1	72.78
1.263	1	-4 4 1	75.19
1.246	1	-4 3 3	76.34
1.238	1	6 0 0	76.98
1.238	1	4 4 -2	76.98
1.226	1	-5 3 1	77.86
1.176	2	-5 3 2	81.86
1.054	1	6 4 1	93.89

Reference

Cruickshank, D.W.J. (1964). Acta Cryst. 17, 677.

de Decker, H.C.J. (1941). Rec. Trav. Chim. 60, 413.

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

Hill, W.L., G.T. Faust, and S.B. Hendricks (1943). J. Am. Chem. Soc. 65, 794.

MacGillavry, C.H., H.C.J. de Decker, and L. M. Nijland (1949). Nature 164, 448.

Potassium Hydrogen Diformate, $KH(HCOO)_2$

Structure

Orthorhombic, Pbca (61), Z=8 [Larsson and Nahringbauer, 1968]

Lattice parameters

a=17.7086 ± 0.0009, b= 7.5096 ± 0.0004, c= 7.3774 ± 0.0004Å
(published value: a=17.7079±.0009Å)[ibid.]

Density

(calculated) 1.76 g/cm^3 [ibid.]

Thermal parameters

Isotropic: K 2.72
O(1) 3.49
O(2) 3.26
O(3) 4.38
O(4) 3.49
C(1) 2.63
C(2) 3.00

Scattering factors

H°, C° [3.3.1A]
O° [3.3.1A] corrected for dispersion by $\Delta f'=0.0$ and $\Delta f''=0.1$ [3.3.2B]
K° [3.3.1A] corrected for dispersion by $\Delta f'=0.3$ and $\Delta f''=1.1$ [3.3.2B]

Scale factor

(integrated intensities) 4.047×10^4

Reference

Larsson, G. and I. Nahringbauer (1968). Acta Cryst. B24, 666.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	$2\theta(^\circ)$ $\lambda = 1.54056$ Å
8.856	100	2 0 0	9.98
5.0464	6	1 1 1	17.56
4.5255	5	2 1 1	19.60
4.4271	1	4 0 0	20.04
3.9277	1	3 1 1	22.62
3.7542	12	0 2 0	23.68
3.6897	1	0 0 2	24.10
3.6100	25	1 0 2	24.64
3.4036	41	2 0 2	26.16
3.3884	44	4 1 1	26.28
3.2877	94	1 2 1	27.10
3.2547	7	1 1 2	27.38
3.1293	41	2 2 1	28.50
3.1016	46	2 1 2	28.76
2.9511	2	6 0 0	30.26
2.9379	7	5 1 1	30.40
2.9117	12	3 2 1	30.68
2.8878	5	3 1 2	30.94
2.8643	3	4 2 0	31.20
2.8342	3	4 0 2	31.54
2.7461	3	6 1 0	32.58
2.6697	28	4 2 1	33.54
2.6513	20	4 1 2	33.78
2.6316	11	0 2 2	34.04
2.6034	3	1 2 2	34.42
2.5744	29	6 1 1	34.82
2.5545	14	5 0 2	35.10
2.5225	45	2 2 2	35.56
2.4326	1	5 2 1	36.92
2.4187	3	5 1 2	37.14
2.4087	12	2 3 0	37.30
2.3493	2	1 3 1	38.28
2.3167	20	1 1 3 +	38.84
2.2895	8	2 3 1	39.32
2.2806	8	7 1 1	39.48
2.2597	3	2 1 3 +	39.86
2.2140	2	8 0 0	40.72
2.2036	2	6 1 2	40.92
2.1792	10	4 3 0	41.40
2.1731	8	3 1 3	41.52
2.1120	3	5 2 2	42.78
2.0897	2	4 3 1	43.26
2.0860	2	7 0 2	43.34
2.0670	8	4 1 3	43.76
2.0571	10	0 2 3 +	43.98
2.0404	18	8 1 1	44.36
2.0171	2	2 3 2 +	44.90
2.0036	1	2 2 3	45.22
1.9545	1	3 3 2	46.42
1.9506	1	5 1 3	46.52

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.9427	3	3 2 3	46.72
1.9088	9	6 3 0	47.60
1.8762	3	4 3 2	48.48
1.8434	3	0 0 4 +	49.40
1.8399	4	8 1 2	49.50
1.8322	7	6 1 3	49.72
1.8192	3	0 4 1	50.10
1.8098	1	1 4 1	50.38
1.8058	2	2 0 4	50.50
1.7879	1	5 3 2	51.04
1.7820	7	2 4 1	51.22
1.7711	1	10 0 0	51.56
1.7553	1	2 1 4	52.06
1.7459	1	1 3 3	52.36
1.7385	2	3 4 1	52.60
1.7361	1	9 0 2	52.68
1.7287	1	4 4 0	52.92
1.7137	1	3 1 4	53.42
1.7025	2	4 0 4	53.80
1.6875	1	6 2 3	54.32
1.6829	4	4 4 1 +	54.48
1.6783	4	10 1 1	54.64
1.6660	1	1 4 2	55.08
1.6483	1	1 2 4	55.72
1.5939	1	3 2 4	57.80
1.5652	1	10 2 1	58.96
1.5504	1	4 2 4	59.58
1.5123	3	8 3 2	61.24
1.5083	2	6 3 3	61.42
1.5052	1	9 1 3	61.56
1.4999	1	5 2 4	61.80
1.4921	3	0 4 3	62.16
1.4904	2	7 0 4	62.24
1.4759	1	12 0 0 +	62.92
1.4717	2	2 4 3	63.12
1.4692	2	10 2 2	63.24
1.4667	2	1 5 1	63.36
1.4467	3	3 4 3 +	64.34
1.4431	3	1 1 5	64.52
1.4399	2	3 3 4	64.68
1.4289	1	2 1 5	65.24
1.4266	1	9 3 2	65.36
1.4113	1	10 1 3	66.16
1.3865	1	1 5 2	67.50
1.3854	1	7 2 4	67.56
1.3750	1	5 4 3	68.14
1.3504	2	12 2 1	69.56
1.3399	1	5 1 5	70.18
1.3386	1	6 5 0	70.26
1.3265	2	6 3 4 +	71.00

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
8.854	83	2 0 0	9.98
5.0447	6	1 1 1	17.57
4.5239	5	2 1 1	19.61
4.4272	1	4 0 0	20.04
3.9282	1	3 1 1	22.62
3.7548	13	0 2 0	23.68
3.6887	1	0 0 2	24.11
3.6112	26	1 0 2	24.63
3.4050	42	2 0 2	26.15
3.3878	41	4 1 1	26.28
3.2881	100	1 2 1	27.10
3.2545	4	1 1 2	27.38
3.1302	45	2 2 1	28.49
3.1011	49	2 1 2	28.76
2.9514	2	6 0 0	30.26
2.9383	7	5 1 1	30.40
2.9111	13	3 2 1	30.69
2.8876	5	3 1 2	30.94
2.8636	9	4 2 0	31.21
2.8339	9	4 0 2	31.54
2.7469	3	6 1 0	32.57
2.6695	31	4 2 1	33.54
2.6514	21	4 1 2	33.78
2.6314	12	0 2 2	34.04
2.6028	3	1 2 2	34.43
2.5742	33	6 1 1	34.82
2.5548	15	5 0 2	35.10
2.5223	52	2 2 2	35.56
2.4324	1	5 2 1	36.92
2.4186	3	5 1 2	37.14
2.4088	14	2 3 0	37.30
2.3495	3	1 3 1	38.28
2.3204	3	6 2 0	38.78
2.3169	22	1 1 3	38.84
2.2898	9	2 3 1	39.31
2.2801	9	7 1 1	39.49
2.2620	1	4 2 2	39.82
2.2596	2	2 1 3	39.86
2.2136	2	8 0 0	40.73
2.2031	2	6 1 2	40.93
2.1790	12	4 3 0	41.40
2.1729	3	3 1 3	41.52
2.1122	3	5 2 2	42.78
2.0898	2	4 3 1	43.26
2.0863	1	7 0 2	43.33
2.0667	10	4 1 3	43.76
2.0573	2	1 3 2	43.98
2.0572	10	0 2 3	43.98
2.0404	22	8 1 1	44.36
2.0180	1	7 2 1	44.88

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
2.0168	1	2 3 2	44.91
2.0038	1	2 2 3	45.21
1.9545	1	3 3 2	46.42
1.9506	1	5 1 3	46.52
1.9426	4	3 2 3	46.72
1.9091	12	6 3 0	47.59
1.8761	3	4 3 2	48.48
1.8443	2	0 0 4	49.37
1.8430	1	9 1 1	49.41
1.8402	4	8 1 2	49.49
1.8322	8	6 1 3	49.72
1.8194	3	0 4 1	50.09
1.8099	1	1 4 1	50.38
1.8056	2	2 0 4	50.50
1.7880	1	5 3 2	51.04
1.7822	8	2 4 1	51.22
1.7709	1	10 0 0	51.57
1.7556	2	2 1 4	52.05
1.7457	1	1 3 3	52.37
1.7387	2	3 4 1	52.59
1.7361	1	9 0 2	52.68
1.7284	1	4 4 0	52.93
1.7140	1	3 1 4	53.41
1.7025	3	4 0 4	53.80
1.6877	1	6 2 3	54.31
1.6828	3	4 4 1	54.48
1.6816	2	3 3 3	54.53
1.6784	3	10 1 1	54.64
1.6657	2	1 4 2	55.09
1.6482	2	1 2 4	55.72
1.6358	1	5 0 4	56.18
1.6097	1	3 4 2	57.18
1.5939	1	3 2 4	57.80
1.5652	2	10 2 1	58.96
1.5506	1	4 2 4	59.57
1.5124	5	8 3 2	61.23
1.5080	1	6 3 3	61.43
1.5052	1	9 1 3	61.56
1.4997	1	5 2 4	61.81
1.4922	4	0 4 3	62.15
1.4903	2	7 0 4	62.24
1.4771	1	7 4 1	62.86
1.4757	1	12 0 0	62.93
1.4715	1	2 4 3	63.13
1.4692	2	10 2 2	63.24
1.4667	1	1 5 1	63.36
1.4480	1	12 1 0	64.28
1.4467	3	3 4 3	64.34
1.4457	1	10 3 0	64.39
1.4430	2	1 1 5	64.53
1.4400	2	3 3 4	64.68
1.4288	1	2 1 5	65.24
1.4266	1	9 3 2	65.36
1.4114	1	10 1 3	66.15
1.3868	1	1 5 2	67.48
1.3852	1	7 2 4	67.57
1.3752	1	5 4 3	68.13
1.3503	2	12 2 1	69.57
1.3401	1	5 1 5	70.17
1.3386	1	6 5 0	70.26
1.3271	2	4 5 2	70.96
1.3264	2	6 3 4	71.00
1.2871	1	12 2 2	73.52
1.2804	1	5 2 5	73.97
1.2711	1	11 3 2	74.60
1.2678	1	1 3 5	74.83
1.2583	1	6 5 2	75.49
1.2340	1	0 6 1	77.25
1.2037	1	3 0 6	79.57
1.1965	1	14 0 2	80.15
1.1890	1	9 4 3	80.76
1.1778	2	8 5 2	81.69
1.1523	1	12 0 4	83.90
1.1461	1	12 4 1	84.46

Potassium Oxalate Perhydrate, $K_2C_2O_4 \cdot H_2O_2$

Structure
Monoclinic, C2/c (15),Z=4. The structure was determined by Pedersen [1967].

Lattice parameters
a=8.969, b=6.532, c=10.955Å, β=108.4° [ibid.]

Density
(calculated) 2.184 g/cm³

Thermal parameters

Isotropic:	K	3.03
	O_1	3.15
	O_p	3.80
	O_2	2.89
	C	2.91

Scattering factors
K^0, C^0, O^{-1} [3.3.1A]

Scale factor
(integrated intensities) 1.490 x 10^4

Reference
Pedersen, B.F. (1967). Acta Chem. Scand. 21, 779.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ λ = 1.54056 Å
5.193	10	0	0	2		17.06
5.041	53	-1	1	1		17.58
4.316	1	1	1	1		20.56
4.255	16	2	0	0		20.86
4.081	21	-1	1	2		21.76
3.962	14	-2	0	2		22.42
3.361	5	1	1	2		26.50
3.266	2	0	2	0		27.28
3.175	34	-1	1	3		28.08
3.116	57	0	2	1		28.62
2.877	72	2	0	2		31.06
2.766	9	0	2	2		32.34
2.715	20	-3	1	1		32.96
2.654	53	-3	1	2	+	33.74
2.636	31	-2	2	1		33.98
2.615	9	-2	0	4		34.26
2.599	72	3	1	0	+	34.48
2.525	54	-1	1	4		35.52
2.520	100	-2	2	2		35.60
2.4075	4	2	2	1		37.32
2.3768	19	0	2	3		37.82
2.3696	12	3	1	1		37.94
2.2974	3	-2	2	3		39.18
2.1812	8	-3	1	4		41.36
2.1592	17	2	2	2	+	41.80
2.1272	7	4	0	0		42.46
2.1092	13	1	3	0		42.84
2.0961	7	3	1	2		43.12
2.0724	7	-1	1	5		43.64
2.0360	4	1	3	1	+	44.46
2.0103	3	-1	3	2		45.06
1.9812	21	-4	0	4		45.76
1.9171	7	-3	1	5		47.38
1.9065	15	2	2	3		47.66
1.9035	21	1	3	2		47.74
1.8675	2	-1	3	3		48.72
1.8406	3	3	1	3	+	49.48
1.8172	1	-2	0	6		50.16
1.8131	4	1	1	5		50.28
1.7991	1	-2	2	5		50.70
1.7892	3	-4	2	3		51.00
1.7827	6	4	2	0		51.20
1.7597	3	-3	3	1		51.92
1.7540	4	0	2	5		52.10
1.7471	3	-1	1	6		52.32
1.7428	3	-3	3	2	+	52.46
1.7096	2	-5	1	1		53.56
1.7043	4	-1	3	4	+	53.74
1.6846	4	4	2	1		54.42
1.6800	3	2	2	4	+	54.58

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.6190	3	3 1 4	56.82
1.6133	2	0 4 1	57.04
1.5878	4	-2 2 6	58.04
1.5858	4	-3 3 4	58.12
1.5784	2	1 3 4	58.42
1.5745	4	-4 2 5	58.58
1.5552	1	5 1 1	59.38
1.5336	2	-2 4 1	60.30
1.5096	3	-2 4 2	61.36
1.5061	5	-1 1 7	61.52
1.4934	5	-6 0 2	62.10
1.4891	3	2 2 5	62.30
1.4844	1	2 4 1	62.52
1.4577	1	-2 4 3	63.80
1.4524	3	2 0 6	64.06
1.4487	2	-4 2 6 +	64.24
1.4391	1	3 3 3	64.72
1.4344	2	3 1 5	64.96
1.4105	2	-2 2 7	66.20
1.3843	4	-5 3 2 +	67.62
1.3603	2	1 1 7 +	68.98
1.3538	1	-6 2 3	69.36
1.3403	2	-6 2 1 +	70.16
1.3376	2	5 1 3	70.32
1.3346	2	-5 3 4	70.50
1.3265	1	-4 2 7	71.00
1.3216	3	-1 1 8 +	71.30
1.3168	2	4 2 4	71.60
1.3076	2	-4 0 8	72.18
1.2901	3	1 3 6	73.32
1.2823	1	-6 2 5	73.84
1.2740	2	1 5 1	74.40
1.2705	2	6 0 2	74.64
1.2562	1	4 4 1	75.64
1.2293	1	-1 5 3	77.60
1.2266	2	5 3 2	77.80
1.2243	1	-6 2 6	77.98
1.2169	1	-5 3 6	78.54
1.2146	1	-2 4 6	78.72
1.2049	1	4 2 5	79.48
1.1969	1	-3 5 1	80.12
1.1934	1	2 2 7	80.40
1.1914	1	-3 1 9	80.56
1.0888	1	0 6 0	90.06
1.0741	1	1 5 5	91.64
1.0614	1	7 3 0	93.06
1.0603	1	-8 2 3	93.18
1.0498	1	-5 5 3	94.40
1.0122	1	5 5 1 +	99.10

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
5.197	11	0 0 2	17.05
5.040	55	-1 1 1	17.58
4.318	1	1 1 1	20.55
4.255	17	2 0 0	20.86
4.083	24	-1 1 2	21.75
3.962	16	-2 0 2	22.42
3.361	6	1 1 2	26.50
3.266	2	0 2 0	27.28
3.176	42	-1 1 3	28.07
3.116	71	0 2 1	28.63
2.877	89	2 0 2	31.06
2.765	11	0 2 2	32.35
2.716	26	-3 1 1	32.95
2.655	46	-3 1 2	33.74
2.654	27	1 1 3	33.74
2.636	36	-2 2 1	33.99
2.615	5	-2 0 4	34.26
2.602	59	3 1 0	34.44
2.599	56	0 0 4	34.48
2.591	3	2 2 0	34.59
2.526	49	-1 1 4	35.52
2.520	100	-2 2 2	35.59
2.4077	5	2 2 1	37.32
2.3766	25	0 2 3	37.82
2.3678	2	3 1 1	37.97
2.2975	4	-2 2 3	39.18
2.1815	10	-3 1 4	41.35
2.1624	1	1 1 4	41.74
2.1590	22	2 2 2	41.81
2.1276	10	4 0 0	42.45
2.1094	17	1 3 0	42.84
2.0964	9	3 1 2	43.11
2.0720	10	-1 1 5	43.65
2.0364	5	1 3 1	44.45
2.0335	2	0 2 4	44.52
2.0101	3	-1 3 2	45.06
1.9810	30	-4 0 4	45.76
1.9173	9	-3 1 5	47.37
1.9066	17	2 2 3	47.66
1.9033	23	1 3 2	47.74
1.8679	3	-1 3 3	48.71
1.8405	2	3 1 3	49.48
1.8400	2	-4 2 1	49.50
1.8174	1	-2 0 6	50.15
1.8128	5	1 1 5	50.29
1.7990	1	-2 2 5	50.70
1.7894	3	-4 2 3	51.00
1.7827	9	4 2 0	51.20
1.7594	5	-3 3 1	51.93
1.7538	4	0 2 5	52.11

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.7472	4	-1 1 6	52.32
1.7424	2	-3 3 2	52.47
1.7422	1	1 3 3	52.48
1.7095	2	-5 1 1	53.56
1.7043	4	-1 3 4	53.74
1.7029	2	-5 1 3	53.79
1.6844	5	4 2 1	54.43
1.6804	1	2 2 4	54.57
1.6801	1	-3 3 3	54.58
1.6192	5	3 1 4	56.81
1.6132	2	0 4 1	57.04
1.5881	5	-2 2 6	58.03
1.5858	4	-3 3 4	58.12
1.5785	2	1 3 4	58.42
1.5747	5	-4 2 5	58.57
1.5550	2	5 1 1	59.39
1.5336	3	-2 4 1	60.30
1.5098	4	-2 4 2	61.35
1.5063	5	-1 1 7	61.51
1.4933	8	-6 0 2	62.10
1.4879	1	2 2 5	62.36
1.4845	2	2 4 1	62.51
1.4772	1	0 4 3	62.86
1.4576	1	-2 4 3	63.80
1.4524	4	2 0 6	64.06
1.4486	1	-4 2 6	64.25
1.4479	1	5 1 2	64.28
1.4393	1	3 3 3	64.71
1.4343	3	3 1 5	64.97
1.4106	3	-2 2 7	66.19
1.3851	1	-2 4 4	67.57
1.3844	7	-5 3 2	67.61
1.3609	2	-3 3 6	68.94
1.3600	2	1 1 7	69.00
1.3538	1	-6 2 3	69.36
1.3410	1	5 3 0	70.12
1.3407	1	2 4 3	70.13
1.3396	2	-6 2 1	70.20
1.3376	1	5 1 3	70.32
1.3346	2	-5 3 4	70.50
1.3265	1	-4 2 7	71.00
1.3219	1	-5 1 7	71.29
1.3217	3	-1 1 8	71.29
1.3207	1	-6 0 6	71.36
1.3166	3	4 2 4	71.61
1.3076	3	-4 0 8	72.18
1.2902	6	1 3 6	73.31
1.2824	2	-6 2 5	73.83
1.2740	4	1 5 1	74.40
1.2703	2	6 0 2	74.66

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.2562	2	4 4 1	75.64
1.2420	1	-7 1 4	76.66
1.2294	3	-1 5 3	77.59
1.2268	2	5 3 2	77.79
1.2244	1	-6 2 6	77.97
1.2170	1	-5 3 6	78.53
1.2147	1	-2 4 6	78.71
1.2050	1	4 2 5	79.47
1.1969	2	-3 5 1	80.12
1.1932	1	2 2 7	80.41
1.1913	1	-3 1 9	80.57
1.1677	1	-7 1 6	82.55
1.1477	1	7 1 1	84.31
1.1295	1	-2 4 7	85.99
1.1163	1	6 2 3	87.27
1.1129	1	-4 2 9	87.60
1.0947	1	-3 5 5	89.44
1.0887	1	0 6 0	90.07
1.0840	1	1 1 9	90.57
1.0795	1	4 4 4	91.05
1.0741	1	1 5 5	91.64
1.0615	1	7 3 0	93.05
1.0604	1	-8 2 3	93.18
1.0558	1	-8 2 4	93.70
1.0498	2	-5 5 3	94.40
1.0153	1	4 4 5	98.69
1.0122	1	5 5 1	99.10
1.0115	1	8 2 0	99.20
1.0000	1	-7 1 9	100.76
.9775	1	-3 3 10	104.00

Structure

Monoclinic, C2/c (15), Z=4 [Lynton and Truter, 1960]

Lattice parameters

a=12.35±.005, b=7.31±.005, c=7.27±.005Å, β= 93°7′±4.5′ [ibid.]

Density

(calculated) 2.58 g/cm^3 [ibid.]

Thermal parameters

Isotropic:	K	1.77
	S	1.12
	O(1)	1.97
	O(2)	2.00
	O(3)	2.02
	O(4)	1.34

Polymorphism

Hähle[1968] described a high-temperature polymorph called the α-form, and confirmed a transition temperature of 330°C.

Scattering factors

K^+, O° [Berghuis et al., 1955]
S° [Tomiie and Stam, 1958]

Scale factor

[integrated intensities] 2.999×10^4

Additional patterns

1. PDF card 1-717 [Hanawalt et al.,1938]
2. PDF 21-683 [Bazarova et al., 1968]
3. Hähle and Meisel,[1968]

Reference

Bazarova, Zh.G., G.K.Boreskov, L.M.Kefeli, L.G. Karakchiev, and A.A. Ostan'kovich. (1968). Proc.Acad.Sci. USSR, Phys. Chem. Sect. (English Transl.) 180, 421.

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Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
6.28	10	1	1	0		14.08
6.16	5	2	0	0		14.36
4.82	46	-1	1	1		18.40
4.687	25	1	1	1		18.92
3.654	47	0	2	0		24.34
3.630	10	0	0	2		24.50
3.581	5	3	1	0		24.84
3.264	100	0	2	1	+	27.30
3.204	77	-2	0	2		27.82
3.153	15	3	1	1		28.28
3.144	14	2	2	0		28.36
3.083	76	4	0	0		28.94
3.056	92	2	0	2		29.20
2.915	44	-2	2	1		30.64
2.855	23	2	2	1		31.30
2.612	16	-3	1	2		34.30
2.576	1	0	2	2		34.80
2.491	7	3	1	2		36.02
2.415	5	-4	0	2		37.20
2.390	6	1	3	0		37.60
2.356	14	4	2	0		38.16
2.345	19	2	2	2		38.36
2.277	4	-1	1	3	+	39.54
2.270	20	-4	2	1		39.68
2.237	6	1	1	3		40.28
2.215	2	4	2	1		40.70
2.191	19	5	1	1		41.16
2.096	12	3	3	0		43.12
2.055	3	6	0	0		44.02
2.051	3	-3	1	3		44.12
2.018	6	0	2	3		44.88
2.006	2	-1	3	2		45.16
1.999	10	3	3	1		45.32
1.987	3	1	3	2		45.62
1.943	29	-2	2	3		46.70
1.940	24	4	2	2		46.80
1.892	11	2	2	3		48.04
1.837	4	-3	3	2		49.58
1.832	3	-6	0	2		49.72
1.814	2	0	0	4		50.24
1.791	2	6	2	0		50.94
1.772	1	0	4	1		51.52
1.767	2	-2	0	4		51.68
1.758	2	-6	2	1	+	51.96
1.748	6	6	0	2		52.28
1.734	4	5	3	0	+	52.76
1.726	6	-5	1	3	+	53.02
1.720	8	6	2	1		53.20
1.709	2	-2	4	1		53.58
1.697	1	2	4	1		53.98

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.687	2	-7 1 1	54.34
1.672	2	5 3 1	54.88
1.654	3	4 2 3	55.50
1.632	1	0 4 2	56.32
1.602	6	-4 0 4	57.46
1.588	4	-5 3 2 +	58.04
1.577	3	6 2 2	58.48
1.573	2	4 4 0	58.66
1.569	1	2 4 2	58.82
1.563	1	3 3 3	59.04
1.553	1	2 2 4	59.46
1.545	2	-4 4 1	59.80
1.541	5	5 3 2	59.96
1.528	3	4 4 1 +	60.56
1.473	2	-6 2 3	63.04
1.470	2	-5 1 4	63.18
1.458	1	0 4 3	63.76
1.448	1	-8 0 2	64.30
1.438	1	1 3 4	64.78
1.430	4	-2 4 3	65.20
1.428	4	7 3 0	65.30
1.425	4	-1 5 1	65.42
1.409	7	2 4 3 +	66.30
1.368	1	-3 1 5	68.52
1.364	5	7 1 3	68.74
1.358	1	-3 5 1	69.12
1.351	5	-6 4 1 +	69.52
1.349	3	-7 3 2 +	69.64
1.345	5	1 5 2	69.86
1.335	1	-4 4 3	70.46
1.312	2	9 1 1	71.92
1.301	1	8 2 2	72.62
1.296	1	-3 5 2	72.96
1.288	1	0 4 4	73.48
1.278	1	-5 3 4	74.12
1.263	2	-5 1 5 +	75.18
1.260	3	-4 2 5	75.40
1.258	1	5 5 0	75.54
1.241	1	9 1 2	76.72
1.233	1	5 5 1	77.30
1.230	1	5 3 4	77.52
1.218	1	0 6 0	78.44
1.214	3	4 2 5 +	78.78
1.204	2	-9 1 3	79.52
1.200	2	-2 0 6	79.90
1.194	3	9 3 0	80.32
1.175	1	2 0 6	81.90
1.172	1	4 4 4 +	82.16
1.151	1	-9 3 2	84.04
1.148	1	0 2 6	84.28

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
6.29	9	1 1 0	14.07
6.17	4	2 0 0	14.35
4.82	44	-1 1 1	18.39
4.689	25	1 1 1	18.91
3.655	51	0 2 0	24.33
3.630	7	0 0 2	24.51
3.583	6	3 1 0	24.83
3.275	29	-3 1 1	27.21
3.265	97	0 2 1	27.30
3.205	85	-2 0 2	27.81
3.182	1	-1 1 2	28.02
3.154	15	3 1 1	28.27
3.144	6	2 2 0	28.36
3.083	82	4 0 0	28.94
3.056	100	2 0 2	29.20
2.915	51	-2 2 1	30.65
2.856	27	2 2 1	31.29
2.613	18	-3 1 2	34.30
2.575	2	0 2 2	34.81
2.492	3	3 1 2	36.02
2.415	6	-4 0 2	37.19
2.390	7	1 3 0	37.60
2.357	17	4 2 0	38.16
2.345	21	2 2 2	38.36
2.280	2	-1 1 3	39.50
2.278	2	-1 3 1	39.53
2.269	24	-4 2 1	39.69
2.259	3	-5 1 1	39.88
2.238	7	1 1 3	40.27
2.215	2	4 2 1	40.71
2.102	25	5 1 1	41.15
2.096	16	3 3 0	43.12
2.055	4	6 0 0	44.02
2.051	1	-3 1 3	44.12
2.018	9	0 2 3	44.89
2.006	1	-1 3 2	45.16
1.999	13	3 3 1	45.33
1.987	3	1 3 2	45.62
1.944	36	-2 2 3	46.69
1.940	13	4 2 2	46.79
1.892	15	2 2 3	48.04
1.837	5	-3 3 2	49.57
1.832	1	-6 0 2	49.74
1.815	3	0 0 4	50.23
1.791	2	6 2 0	50.93
1.772	2	0 4 1	51.53
1.767	2	-2 0 4	51.68
1.759	2	-6 2 1	51.95
1.757	1	-1 1 4	52.01
1.748	9	6 0 2	52.29

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.733	5	5 3 0	52.77
1.731	1	1 1 4	52.85
1.726	5	-5 1 3	53.01
1.724	5	-4 2 3	53.06
1.720	7	6 2 1	53.20
1.713	1	7 1 0	53.46
1.709	2	-2 4 1	53.57
1.697	1	2 4 1	53.98
1.687	2	-7 1 1	54.34
1.672	3	5 3 1	54.88
1.654	5	4 2 3	55.50
1.632	1	0 4 2	56.32
1.607	1	-3 3 3	57.30
1.603	8	-4 0 4	57.46
1.588	3	-5 3 2	58.04
1.588	3	-2 4 2	58.05
1.577	4	6 2 2	58.47
1.572	1	4 4 0	58.68
1.568	1	2 4 2	58.83
1.563	1	3 3 3	59.05
1.553	1	2 2 4	59.46
1.545	3	-4 4 1	59.80
1.541	5	5 3 2	59.96
1.528	2	4 0 4	60.54
1.528	3	4 4 1	60.56
1.474	3	-6 2 3	63.03
1.471	2	-5 1 4	63.18
1.458	2	0 4 3	63.77
1.447	2	-8 0 2	64.31
1.438	1	1 3 4	64.77
1.430	5	-2 4 3	65.20
1.428	5	7 3 0	65.31
1.425	2	-1 5 1	65.42
1.409	2	2 4 3	66.29
1.408	2	6 2 3	66.32
1.407	2	-8 2 1	66.37
1.368	1	-3 1 5	68.52
1.364	7	7 1 3	68.75
1.358	1	-3 5 1	69.12
1.354	1	3 3 4	69.37
1.351	5	-6 4 1	69.52
1.351	1	-1 5 2	69.52
1.349	5	0 2 5	69.62
1.349	7	-7 3 2	69.64
1.349	1	3 5 1	69.65
1.345	1	1 5 2	69.88
1.335	1	-4 4 3	70.46
1.324	1	3 1 5	71.16
1.312	4	9 1 1	71.93
1.301	1	8 2 2	72.63
1.296	2	-3 5 2	72.95
1.288	1	0 4 4	73.48
1.278	1	-5 3 4	74.12
1.270	1	-2 4 4	74.65
1.263	1	6 4 2	75.14
1.263	3	-5 1 5	75.18
1.260	3	-4 2 5	75.39
1.258	1	5 5 0	75.54
1.241	2	9 1 2	76.72
1.233	2	5 5 1	77.29
1.230	1	5 3 4	77.53
1.218	2	0 6 0	78.43
1.214	1	7 1 4	78.77
1.214	4	4 2 5	78.78
1.204	3	-9 1 3	79.51
1.200	2	-2 0 6	79.90
1.194	4	9 3 0	80.32
1.188	1	3 5 3	80.85
1.175	1	2 0 6	81.91
1.172	1	4 4 4	82.16
1.171	1	6 4 3	82.23
1.151	1	-9 3 2	84.03
1.149	1	0 2 6	84.23
1.140	1	-2 2 6	85.03
1.139	2	-2 6 2	85.12
1.138	3	-7 1 5	85.24
1.137	1	-1 5 4	85.27
1.137	4	0 4 5	85.31
1.133	3	4 6 0	85.66
1.132	3	2 6 2	85.78
1.130	2	1 5 4	85.93
1.129	1	-5 5 3	86.06
1.119	1	9 3 2	87.02
1.118	3	-7 5 1	87.13
1.108	1	11 1 0	88.07
1.104	2	-11 1 1	88.46
1.099	1	7 3 4	89.02

Rubidium Oxalate Perhydrate, $Rb_2C_2O_4 \cdot H_2O_2$

Structure
Monoclinic, C2/c (15),Z=4. The structure was determined by Pedersen [1967].

Lattice parameters
a=9.251, b=6.808, c=11.199Å, β=107.45° [ibid.]

Density
(calculated) 2.892 g/cm³

Thermal parameters

Isotropic:	Rb	3.95
	O_1	4.61
	O_p	5.04
	O_2	3.72
	C	4.30

Scattering factors
C^0, Rb^0, O^{-1} [3.3.1A]

Scale factor
(integrated intensities) 4.195 x 10^4

Reference
Pedersen, B.F. (1967). Acta Chem. Scand. 21, 779.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				$2\theta(°)$ $\lambda = 1.54056$ Å
5.388	19	1	1	0		16.44
5.211	22	-1	1	1		17.00
4.494	77	1	1	1		19.74
4.414	16	2	0	0		20.10
4.199	33	-1	1	2		21.14
4.051	66	-2	0	2		21.92
3.488	2	1	1	2		25.52
3.404	12	0	2	0		26.16
3.257	85	-1	1	3		27.36
3.243	100	0	2	1		27.48
2.990	83	2	0	2		29.86
2.870	3	0	2	2		31.14
2.808	52	-3	1	1		31.84
2.748	17	1	1	3		32.56
2.735	55	-2	2	1	+	32.72
2.701	39	3	1	0	+	33.14
2.671	50	0	0	4	+	33.52
2.606	56	-2	2	2		34.38
2.589	32	-1	1	4		34.62
2.506	9	2	2	1		35.80
2.4610	24	0	2	3	+	36.48
2.3684	9	-2	2	3		37.96
2.2962	1	-4	0	2		39.20
2.2468	17	2	2	2		40.10
2.2308	8	-3	1	4		40.40
2.2067	14	4	0	0		40.86
2.1974	19	1	3	0		41.04
2.1802	4	3	1	2		41.38
2.1243	5	-1	1	5	+	42.52
2.1008	5	0	2	4		43.02
2.0878	7	-1	3	2		43.30
2.0248	20	-4	0	4		44.72
1.9812	36	1	3	2	+	45.76
1.9585	13	-3	1	5		46.32
1.9364	1	-1	3	3		46.88
1.9133	6	3	1	3		47.48
1.9073	5	-4	2	1		47.64
1.8725	7	1	1	5		48.58
1.8553	5	-2	0	6		49.06
1.8511	10	4	2	0	+	49.18
1.8469	8	-2	2	5		49.30
1.8434	8	-4	2	3		49.40
1.8274	2	-3	3	1		49.86
1.8098	7	0	2	5		50.38
1.8058	7	-3	3	2		50.50
1.7971	5	3	3	0		50.76
1.7919	4	-1	1	6		50.92
1.7846	1	-5	1	2		51.14
1.7692	2	-5	1	1		51.62
1.7628	7	-1	3	4		51.82

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.7515	12	4 2 1 +	52.18
1.7404	2	-4 2 4	52.54
1.7197	1	-3 1 6	53.22
1.6812	6	3 1 4 +	54.54
1.6359	5	-3 3 4 +	56.18
1.6295	4	-2 2 6 +	56.42
1.6148	7	-4 2 5 +	56.98
1.6055	1	1 1 6	57.34
1.5959	4	-2 4 1	57.72
1.5691	2	-2 4 2	58.80
1.5443	6	-1 1 7	59.84
1.5410	7	-6 0 2 +	59.98
1.5373	3	0 4 3	60.14
1.5123	2	-2 4 3	61.24
1.5052	1	5 1 2	61.56
1.5021	3	2 0 6	61.70
1.4951	2	4 0 4	62.02
1.4882	2	3 1 5	62.34
1.4793	1	2 4 2	62.76
1.4467	2	-2 2 7	64.34
1.4336	5	-5 3 2 +	65.00
1.4026	2	1 1 7 +	66.62
1.3993	3	-3 3 6	66.80
1.3956	3	2 4 3 +	67.00
1.3916	2	5 1 3 +	67.22
1.3879	3	-6 2 1	67.42
1.3786	2	3 3 4	67.94
1.3757	2	-5 3 4	68.10
1.3686	2	4 2 4	68.50
1.3572	1	-4 2 7	69.16
1.3555	2	-1 1 8	69.26
1.3497	3	-5 1 7 +	69.60
1.3460	2	-2 4 5 +	69.82
1.3446	2	-4 4 3	69.90
1.3356	4	1 3 6 +	70.44
1.3323	3	-4 0 8 +	70.64
1.3278	3	1 5 1	70.92
1.3203	1	6 0 2	71.38
1.3168	2	-6 2 5	71.60
1.3076	2	4 4 1	72.18
1.2781	2	-1 5 3 +	74.12
1.2764	3	5 3 2 +	74.24
1.2545	1	-6 2 6 +	75.76
1.2520	2	4 2 5	75.94
1.2503	1	-5 3 6	76.06
1.2475	1	-4 4 5	76.26
1.2456	2	-3 5 1	76.40
1.2431	2	-7 1 5	76.58
1.2347	1	2 2 7	77.20
1.2172	1	-3 1 9	78.52

Calculated Pattern *(Integrated)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
5.390	19	1 1 0	16.43
5.212	22	-1 1 1	17.00
4.493	83	1 1 1	19.74
4.413	16	2 0 0	20.11
4.198	36	-1 1 2	21.14
4.050	75	-2 0 2	21.93
3.488	2	1 1 2	25.51
3.404	13	0 2 0	26.16
3.258	96	-1 1 3	27.35
3.243	100	0 2 1	27.48
2.990	98	2 0 2	29.86
2.871	3	0 2 2	31.13
2.808	62	-3 1 1	31.84
2.749	18	1 1 3	32.55
2.735	49	-2 2 1	32.72
2.732	39	-3 1 2	32.76
2.700	47	3 1 0	33.15
2.695	3	2 2 0	33.21
2.671	61	0 0 4	33.52
2.666	1	-2 0 4	33.58
2.606	70	-2 2 2	34.39
2.589	37	-1 1 4	34.61
2.507	12	2 2 1	35.79
2.4620	3	3 1 1	36.46
2.4607	28	0 2 3	36.48
2.3679	12	-2 2 3	37.97
2.2966	1	-4 0 2	39.19
2.2465	22	2 2 2	40.11
2.2306	9	-3 1 4	40.40
2.2063	18	4 0 0	40.87
2.1978	22	1 3 0	41.03
2.1804	5	3 1 2	41.38
2.1241	7	-1 1 5	42.52
2.1217	1	1 3 1	42.57
2.1013	6	0 2 4	43.01
2.0881	9	-1 3 2	43.29
2.0310	1	2 0 4	44.58
2.0251	28	-4 0 4	44.71
1.9816	23	2 2 3	45.75
1.9811	28	1 3 2	45.76
1.9584	18	-3 1 5	46.32
1.9361	1	-1 3 3	46.89
1.9131	8	3 1 3	47.49
1.9068	4	-4 2 1	47.65
1.8724	10	1 1 5	48.59
1.8556	6	-2 0 6	49.05
1.8526	2	4 0 2	49.14
1.8514	9	4 2 0	49.17
1.8472	3	-2 2 5	49.29
1.8435	9	-4 2 3	49.40

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.8275	2	-3 3 1	49.86
1.8097	9	0 2 5	50.38
1.8060	5	-3 3 2	50.49
1.7968	6	3 3 0	50.77
1.7913	3	-1 1 6	50.94
1.7846	1	-5 1 2	51.14
1.7691	2	-5 1 1	51.62
1.7629	10	-1 3 4	51.82
1.7516	10	4 2 1	52.18
1.7514	7	-5 1 3	52.18
1.7404	2	-4 2 4	52.54
1.7200	1	-3 1 6	53.21
1.6816	5	3 1 4	54.53
1.6808	4	0 4 1	54.55
1.6382	2	1 3 4	56.10
1.6361	7	-3 3 4	56.17
1.6292	5	-2 2 6	56.43
1.6272	1	4 2 2	56.51
1.6160	1	3 3 2	56.94
1.6156	5	5 1 1	56.95
1.6147	6	-4 2 5	56.98
1.6054	1	1 1 6	57.34
1.5960	6	-2 4 1	57.72
1.5691	4	-2 4 2	58.80
1.5466	3	2 4 1	59.74
1.5445	7	-1 1 7	59.83
1.5425	1	2 2 5	59.92
1.5413	7	-6 0 2	59.97
1.5356	2	0 4 3	60.21
1.5123	3	-2 4 3	61.24
1.5055	2	5 1 2	61.55
1.5023	5	2 0 6	61.69
1.4951	2	4 0 4	62.02
1.4881	3	3 1 5	62.35
1.4792	1	2 4 2	62.77
1.4709	1	6 0 0	63.16
1.4465	4	-2 2 7	64.35
1.4370	1	-1 3 6	64.83
1.4353	1	0 4 4	64.91
1.4336	7	-5 3 2	65.00
1.4041	1	-6 2 2	66.54
1.4027	2	1 1 7	66.62
1.3994	3	-3 3 6	66.79
1.3963	1	-6 2 3	66.96
1.3954	3	2 4 3	67.01
1.3932	1	5 3 0	67.13
1.3910	2	5 1 3	67.25
1.3879	4	-6 2 1	67.42
1.3785	3	3 3 4	67.94
1.3760	2	-5 3 4	68.08

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.3689	3	4 2 4	68.49
1.3572	2	-4 2 7	69.16
1.3555	2	-1 1 8	69.26
1.3501	2	-6 0 6	69.58
1.3494	3	-5 1 7	69.62
1.3476	1	4 4 0	69.72
1.3460	1	-2 4 5	69.82
1.3445	2	-4 4 3	69.90
1.3356	6	1 3 6	70.44
1.3355	1	0 0 8	70.45
1.3332	3	-4 0 8	70.59
1.3313	2	0 4 5	70.70
1.3276	5	1 5 1	70.93
1.3204	2	6 0 2	71.38
1.3168	3	-6 2 5	71.60
1.3076	3	4 4 1	72.18
1.2783	3	-1 5 3	74.11
1.2775	1	-7 1 4	74.17
1.2764	3	5 3 2	74.24
1.2752	1	-7 1 1	74.32
1.2550	1	-6 2 6	75.73
1.2543	1	-2 4 6	75.78
1.2520	2	4 2 5	75.94
1.2502	1	-5 3 6	76.06
1.2476	1	-4 4 5	76.25
1.2455	2	-3 5 1	76.41
1.2431	1	-7 1 5	76.58
1.2347	2	2 2 7	77.20
1.2171	1	-3 1 9	78.52
1.1952	1	3 1 7	80.25
1.1918	1	7 1 1	80.53
1.1811	1	-1 3 8	81.41
1.1650	1	-2 4 7	82.78
1.1610	2	6 2 3	83.13
1.1378	1	-4 2 9	85.21
1.1347	1	0 6 0	85.51
1.1333	1	-3 5 5	85.63
1.1284	1	-7 3 4	86.10
1.1243	1	3 5 3	86.49
1.1209	1	0 2 9	86.82
1.1171	1	1 1 9	87.19
1.1159	2	1 5 5	87.30
1.1033	1	-5 3 8	88.55
1.1021	2	7 3 0	88.68
1.0949	1	-8 2 3	89.42
1.0939	1	-6 4 5	89.52
1.0886	2	-5 5 3	90.08
1.0608	1	2 6 2	93.12
1.0559	1	4 4 5	93.69
1.0535	1	5 5 1	93.96

Structure
Cubic, Im3m (229),Z=2. The structure was determined by Hull [1917].

Lattice parameters
a = 4.2908 Å ± .0005. (published value, a = 4.2906 Å ±.0005) [Aruja and Perlitz, 1939].

Density
(calculated) 0.966 g/cm^3

Thermal parameters
Isotropic, overall B=2.0

Polymorphism
Sodium has a face-centered cubic structure at -195 °C [Barrett, 1948].

Scattering factors
Na° [3.3.1A]

Scale factor
(integrated intensities) 0.09447 x 10^4

Additional patterns
1. PDF card 1-850 [Hanawalt et al.,1938]
2. Hull [1917]

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
3.0335	100	1 1 0	29.42
2.1455	15	2 0 0	42.08
1.7515	23	2 1 1	52.18
1.5172	5	2 2 0	61.02
1.3568	6	3 1 0 +	69.18
1.2387	1	2 2 2	76.90
1.1467	4	3 2 1 +	84.40
1.0113	2	4 1 1 +	99.22
.9595	1	4 2 0 +	106.80
.8415	1	4 3 1 +	132.52
.7834	1	5 2 1 +	159.00

Calculated Pattern *(Integrated)*

d (Å)	*I*	*hkl*	*2θ(°)* λ = 1.54056 Å
3.0341	100	1 1 0	29.41
2.1454	16	2 0 0	42.08
1.7517	29	2 1 1	52.17
1.5170	8	2 2 0	61.03
1.3569	4	3 1 0	69.18
1.3569	4	0 1 3	69.18
1.2386	2	2 2 2	76.91
1.1468	4	3 2 1	84.40
1.1468	4	1 2 3	84.40
1.0113	1	3 3 0	99.22
1.0113	2	4 1 1	99.22
.9594	1	4 2 0	106.80
.9594	1	0 2 4	106.80
.9148	1	3 3 2	114.71
.8759	1	4 2 2	123.15
.8415	1	4 3 1	132.52
.8415	1	1 3 4	132.52
.7834	2	1 2 5	159.01
.7834	2	5 2 1	159.01

Reference

Aruja, E.and H. Perlitz (1939). Z. Krist. 100, 195.
Barrett, C.S. (1948). Am. Mineralogist 33, 749.
Hanawalt, J.D., H.W. Rinn, and L.K. Frevel (1938). Ind. Eng. Chem. Anal.Ed.10, 457.
Hull, A. W. (1917). Phys. Rev. 10, 661.

Structure
Orthorhombic, Fdd2 (43), Z=8. The structure was determined by Corazza and Sabelli [1967].

Lattice parameters
a=11.32±0.02, b=20.06±0.02, c=6.00±0.02Å [Evans, 1948]

Density
(calculated) 2.360 g/cm^3

Thermal parameters
Isotropic [Corazza and Sabelli,1967]

Scattering factors
H°,Na°,Ca°,C°,O° [Cromer and Waber,1965]

Scale factor
(integrated intensities) 6.393 x 10^4

Additional patterns
1. PDF card 2-1051 [Dow Chemical Co., Midland, Michigan]
2. PDF card 22-476 [Fahey and Mrose, 1962]

Reference
Corazza,E. and C. Sabelli(1967).Acta Cryst. 23, 763.
Cromer, D.T. and J.T. Waber (1965). Acta Cryst. 18, 104.
Evans, H.T.,Jr. (1948). Am. Mineralogist 33, 261.
Fahey, J.J. and M.E. Mrose (1962). U.S. Geol. Surv. Profess. Paper 405, 1.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*				2θ(°) λ = 1.54056 Å
5.12	100	1	1	1		17.30
5.01	40	0	4	0		17.68
4.93	74	2	2	0		17.98
4.15	14	1	3	1		21.38
3.75	3	2	4	0		23.68
3.20	40	1	5	1		27.86
3.16	58	3	1	1		28.26
2.88	49	3	3	1	+	31.00
2.88	41	0	2	2		31.08
2.83	7	4	0	0		31.58
2.72	53	4	2	0		32.86
2.65	91	2	0	2		33.78
2.56	93	2	2	2		34.98
2.52	33	1	7	1		35.58
2.51	77	0	8	0		35.78
2.50	81	3	5	1		35.90
2.34	8	2	4	2		38.38
2.29	28	2	8	0		39.26
2.23	4	0	6	2		40.36
2.16	12	4	6	0		41.78
2.13	53	3	7	1		42.34
2.11	36	5	1	1		42.90
2.08	3	2	6	2		43.54
2.05	15	1	9	1		44.04
2.02	64	4	2	2	+	44.92
1.960	1	1	1	3		46.28
1.890	21	2	10	0	+	48.10
1.877	10	4	8	0		48.46
1.873	9	5	5	1		48.58
1.854	12	6	2	0		49.10
1.827	5	3	9	1		49.86
1.821	30	2	8	2		50.04
1.768	48	1	5	3	+	51.66
1.763	28	3	1	3		51.82
1.753	8	4	6	2		52.14
1.725	4	1	11	1		53.06
1.708	13	3	3	3		53.60
1.704	17	5	7	1		53.76
1.668	9	0	10	2		55.02
1.643	4	6	6	0		55.92
1.636	4	4	10	0		56.16
1.623	5	1	7	3		56.66
1.603	3	2	12	0		57.44
1.599	7	2	10	2		57.58
1.597	4	6	0	2		57.68
1.591	2	4	8	2		57.90
1.584	1	3	11	1		58.20
1.577	3	6	2	2		58.46
1.557	6	7	1	1		59.32
1.535	5	5	9	1		60.22

Sodium Calcium Carbonate Hydrate, pirssonite, $Na_2Ca(CO_3)_2 \cdot 2H_2O$ – continued

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.522	13	6 4 2 +	60.82
1.507	2	6 8 0	61.46
1.504	6	3 7 3	61.62
1.500	6	0 0 4	61.78
1.463	6	5 3 3	63.56
1.455	2	7 5 1	63.92
1.441	5	6 6 2	64.62
1.437	11	4 10 2 +	64.84
1.415	3	8 0 0 +	65.96
1.393	2	2 4 4	67.14
1.389	7	3 13 1	67.34
1.386	4	3 9 3	67.54
1.382	2	5 11 1	67.74
1.374	2	6 10 0	68.18
1.371	2	7 7 1	68.36
1.362	3	8 4 0	68.90
1.330	2	2 6 4	70.76
1.314	4	4 2 4	71.78
1.297	6	1 15 1 +	72.88
1.287	1	0 8 4	73.50
1.281	4	4 4 4	73.90
1.279	8	7 9 1 +	74.08
1.269	1	3 11 3	74.74
1.260	2	2 14 2	75.34
1.255	3	7 1 3	75.72
1.254	2	0 16 0	75.80
1.247	1	5 13 1	76.28
1.244	2	5 9 3	76.52
1.236	1	7 3 3	77.12
1.234	3	3 15 1	77.28
1.232	3	4 6 4	77.38
1.229	4	9 1 1	77.64
1.215	5	1 13 3	78.72
1.200	2	7 5 3	79.88
1.195	3	8 6 2	80.26
1.186	2	7 11 1	81.00
1.176	2	4 14 2	81.86
1.175	2	2 10 4	81.90
1.172	2	4 8 4	82.20
1.166	1	6 2 4	82.68
1.162	2	3 13 3	83.02
1.158	2	5 11 3	83.40
1.155	4	6 12 2	83.68
1.152	3	7 7 3	83.96
1.146	1	4 16 0	84.44
1.144	4	1 5 5 +	84.68
1.141	3	6 14 0 +	84.92
1.133	2	2 16 2	85.64
1.127	4	3 3 5	86.22
1.106	4	1 15 3 +	88.24
1.100	2	3 5 5	88.92
1.095	1	7 9 3	89.38
1.093	2	2 18 0	89.58
1.080	1	8 12 0	91.00
1.078	3	0 9 1	91.26
1.075	2	5 13 3	91.54
1.063	1	9 1 3	92.84
1.062	1	3 7 5	92.98
1.059	1	10 0 2	93.32
1.047	2	5 3 5	94.72
1.038	4	4 12 4	95.76
1.036	4	10 4 2 +	96.06
1.031	2	5 17 1	96.70
1.029	1	9 5 3	96.92
1.028	1	2 18 2	97.04
1.020	1	9 11 1	98.04
1.019	1	2 14 4	98.18
1.013	2	11 1 1 +	99.00
1.010	2	10 6 2	99.44
1.008	5	8 4 4	99.62
1.003	2	3 19 1 +	100.40
.998	1	5 15 3	101.04
.995	1	0 2 6	101.44
.985	1	2 0 6	102.92
.983	1	11 5 1	103.12
.980	3	4 18 2 +	103.62
.976	1	10 8 2	104.28
.975	1	7 13 3	104.40
.962	2	0 16 4 +	106.38
.960	1	6 18 0	106.78
.957	1	5 9 5 +	107.14
.956	1	11 7 1	107.34
.955	2	8 14 2	107.60
.952	1	8 8 4	108.00
.945	1	5 19 1	109.24
.944	1	1 13 5	109.38
.941	2	7 17 1	109.80
.940	1	1 21 1	110.04
.939	1	4 2 6	110.28
.938	1	2 20 2	110.38
.936	1	10 10 2	110.68
.919	1	3 13 5 +	113.94
.917	3	2 8 6 +	114.36
.908	2	6 14 4 +	116.04
.906	1	9 15 1	116.52
.896	1	12 2 2	118.50
.895	2	0 10 6 +	118.80
.890	1	1 15 5	119.80
.886	1	11 11 1	120.70
.886	1	6 20 0	120.86

Calculated Pattern *(Integrated)*			
d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
5.13	90	1 1 1	17.29
5.01	34	0 4 0	17.67
4.93	64	2 2 0	17.98
4.15	13	1 3 1	21.37
3.75	3	2 4 0	23.68
3.20	41	1 5 1	27.86
3.15	61	3 1 1	28.27
2.88	47	3 3 1	31.00
2.88	3	2 6 0	31.04
2.87	12	0 2 2	31.09
2.83	8	4 0 0	31.59
2.72	55	4 2 0	32.86
2.65	100	2 0 2	33.79
2.56	93	2 2 2	34.98
2.52	31	1 7 1	35.58
2.51	74	0 8 0	35.78
2.50	60	3 5 1	35.91
2.34	9	2 4 2	38.38
2.29	32	2 8 0	39.27
2.23	4	0 6 2	40.36
2.16	14	4 6 0	41.78
2.13	61	3 7 1	42.34
2.11	40	5 1 1	42.90
2.08	3	2 6 2	43.54
2.05	17	1 9 1	44.04
2.02	19	5 3 1	44.85
2.02	68	4 2 2	44.91
1.960	2	1 1 3	46.28
1.891	16	2 10 0	48.08
1.889	15	1 3 3	48.12
1.877	11	4 8 0	48.46
1.873	4	5 5 1	48.56
1.854	14	6 2 0	49.09
1.828	4	3 9 1	49.85
1.822	38	2 8 2	50.03
1.768	60	1 5 3	51.66
1.766	1	6 4 0	51.72
1.760	4	3 1 3	51.90
1.753	9	4 6 2	52.13
1.724	5	1 11 1	53.06
1.708	16	3 3 3	53.60
1.703	15	5 7 1	53.77
1.668	11	0 10 2	55.02
1.643	5	6 6 0	55.91
1.637	5	4 10 0	56.16
1.623	7	1 7 3	56.66
1.603	3	2 12 0	57.43
1.600	7	2 10 2	57.57
1.597	2	6 0 2	57.67
1.591	2	4 8 2	57.91

d (Å)	*I*	*hkl*	2θ(°) λ = 1.54056 Å
1.584	1	3 11 1	58.21
1.577	4	6 2 2	58.47
1.557	9	7 1 1	59.31
1.535	6	5 9 1	60.22
1.522	24	6 4 2	60.82
1.521	1	7 3 1	60.87
1.508	1	6 8 0	61.45
1.504	7	3 7 3	61.61
1.500	4	0 0 4	61.80
1.463	8	5 3 3	63.56
1.455	2	7 5 1	63.92
1.441	7	6 6 2	64.62
1.437	3	0 4 4	64.82
1.437	11	4 10 2	64.84
1.435	4	2 2 4	64.93
1.415	4	8 0 0	65.96
1.414	1	2 12 2	66.02
1.393	3	2 4 4	67.15
1.389	9	3 13 1	67.34
1.385	1	3 9 3	67.60
1.382	3	5 11 1	67.75
1.374	3	6 10 0	68.18
1.371	1	7 7 1	68.36
1.362	5	8 4 0	68.89
1.338	1	1 11 3	70.29
1.330	3	2 6 4	70.77
1.314	5	4 2 4	71.78
1.298	1	4 12 2	72.82
1.297	8	1 15 1	72.89
1.287	2	0 8 4	73.51
1.281	5	4 4 4	73.90
1.279	10	7 9 1	74.07
1.278	1	4 14 0	74.11
1.269	1	3 11 3	74.74
1.260	3	2 14 2	75.34
1.255	4	7 1 3	75.72
1.254	2	0 16 0	75.81
1.247	2	5 13 1	76.28
1.244	2	5 9 3	76.53
1.236	2	7 3 3	77.11
1.234	4	3 15 1	77.28
1.232	2	4 6 4	77.39
1.229	5	9 1 1	77.64
1.215	8	1 13 3	78.71
1.200	4	7 5 3	79.87
1.195	4	8 6 2	80.25
1.186	3	7 11 1	81.00
1.176	2	4 14 2	81.84
1.175	2	2 10 4	81.91
1.172	2	4 8 4	82.20

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
1.166	2	6 2 4	82.68
1.162	4	3 13 3	83.01
1.158	3	5 11 3	83.40
1.155	6	6 12 2	83.68
1.152	2	7 7 3	83.97
1.146	1	4 16 0	84.44
1.144	4	1 5 5	84.67
1.143	2	6 4 4	84.72
1.142	1	3 1 5	84.86
1.141	1	6 14 0	84.92
1.133	3	2 16 2	85.63
1.127	6	3 3 5	86.21
1.116	1	0 12 4	87.25
1.108	3	6 6 4	88.11
1.107	3	3 17 1	88.20
1.106	5	1 15 3	88.25
1.106	1	4 10 4	88.31
1.100	2	3 5 5	88.92
1.095	2	7 9 3	89.39
1.093	2	2 18 0	89.57
1.080	2	8 12 0	90.99
1.079	1	8 10 2	91.11
1.078	5	9 9 1	91.26
1.075	1	5 13 3	91.52
1.063	1	9 1 3	92.85
1.062	1	3 7 5	92.98
1.059	2	10 0 2	93.32
1.053	1	10 2 2	94.00
1.047	3	5 3 5	94.71
1.039	7	4 12 4	95.75
1.036	4	10 4 2	96.03
1.035	2	7 11 3	96.16
1.031	4	5 17 1	96.70
1.029	1	9 5 3	96.92
1.027	1	2 18 2	97.14
1.024	1	8 2 4	97.58
1.020	2	9 11 1	98.04
1.019	1	2 14 4	98.19
1.013	2	11 1 1	99.00
1.012	1	1 17 3	99.10
1.010	2	10 6 2	99.44
1.008	10	8 4 4	99.63
1.003	1	0 20 0	100.34
1.003	1	11 3 1	100.37
1.002	2	3 19 1	100.42
.998	1	5 15 3	101.05
.995	1	0 2 6	101.45
.985	2	2 0 6	102.93
.983	1	11 5 1	103.13
.980	4	4 18 2	103.62

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
.980	2	2 2 6	103.62
.976	1	10 8 2	104.28
.975	1	7 13 3	104.41
.969	1	3 11 5	105.32
.966	1	2 4 6	105.72
.963	1	7 1 5	106.31
.962	1	9 13 1	106.35
.962	2	0 16 4	106.40
.960	1	6 18 0	106.79
.958	1	0 6 6	107.03
.957	1	5 9 5	107.12
.956	2	11 7 1	107.34
.954	3	8 14 2	107.61
.952	1	8 8 4	107.99
.945	1	5 19 1	109.21
.944	3	1 13 5	109.37
.941	2	7 17 1	109.81
.940	1	1 21 1	110.04
.939	1	4 2 6	110.28
.938	1	2 20 2	110.39
.937	1	10 10 2	110.66
.927	1	5 17 3	112.36
.923	1	11 9 1	113.10
.919	1	9 11 3	113.80
.919	1	3 13 5	113.94
.917	2	5 11 5	114.36
.917	3	2 8 6	114.36
.916	1	7 15 3	114.45
.908	3	6 14 4	116.03
.907	2	4 6 6	116.17
.906	1	9 15 1	116.52
.900	1	10 2 4	117.73
.896	2	12 2 2	118.50
.895	3	0 10 6	118.79
.895	2	10 12 2	118.85
.890	1	1 15 5	119.79
.889	1	10 4 4	120.04
.886	1	11 11 1	120.68
.886	1	6 20 0	120.86
.884	1	2 18 4	121.33
.883	3	12 8 0	121.48
.876	2	8 12 4	123.01
.875	2	7 19 1	123.46
.874	1	5 13 5	123.64
.872	3	10 6 4	124.03
.870	4	6 4 6	124.56
.869	1	3 15 5	124.81
.869	1	12 6 2	124.86
.867	1	9 1 5	125.25
.863	1	5 19 3	126.35

Structure
Orthorhombic, Cmca (64), Z=8. The structure was determined by Seleborg [1967].

Lattice parameters
a=7.164±0.006, b=11.837±0.004, c=14.714±0.002Å.(published value: c=14.713±.002Å)

Density
(calculated) 3.725 g/cm^3

Thermal parameters
Isotropic [ibid.]

Scattering factors
Na^+, Mo^{3+}, O^{-1} [3.3.1A]. The values for Na^+ and Mo^{3+} were corrected for the real part of the dispersion correction, using $\Delta f=0.1$ and $\Delta f=-0.5$ for the sodium and molybdenum respectively.

Scale factor
(integrated intensities) 32.52 x 10^4

Reference
Seleborg, M. (1967). Acta Chem. Scand.21, 499.

Calculated Pattern *(Peak heights)*

d (Å)	I	hkl	2θ(°) λ = 1.54056 Å
7.36	30	0 0 2	12.02
5.92	12	0 2 0	14.96
5.65	4	1 1 1	15.66
5.49	100	0 2 1	16.14
4.706	91	1 1 2	18.84
4.609	44	0 2 2	19.24
3.828	3	1 1 3	23.22
3.776	54	0 2 3	23.54
3.678	6	0 0 4	24.18
3.363	2	1 3 1	26.48
3.220	68	2 0 2	27.68
3.153	66	1 1 4	28.28
3.125	82	0 2 4 +	28.54
3.064	92	2 2 0	29.12
3.000	35	2 2 1	29.76
2.959	9	0 4 0	30.18
2.901	15	0 4 1	30.80
2.829	1	2 2 2	31.60
2.746	10	0 4 2	32.58
2.635	14	0 2 5	34.00
2.599	11	2 2 3	34.48
2.566	19	2 0 4	34.94
2.534	13	0 4 3	35.40
2.518	11	1 3 4	35.62
2.452	3	0 0 6	36.62
2.354	1	2 2 4	38.20
2.305	21	0 4 4	39.04
2.265	3	0 2 6	39.76
2.254	6	2 4 1	39.96
2.231	4	3 1 2	40.40
2.222	3	1 5 1	40.56
2.149	16	1 5 2	42.00
2.122	6	2 2 5	42.56
2.113	2	3 1 3	42.76
2.087	5	0 4 5	43.32
2.069	10	2 4 3	43.72
2.043	2	1 5 3	44.30
2.024	2	3 3 1 +	44.74
1.988	2	1 1 7	45.60
1.980	9	0 2 7	45.78
1.975	24	3 1 4 +	45.92
1.969	15	3 3 2	46.06
1.939	1	2 4 4	46.82
1.915	13	2 2 6	47.44
1.906	4	0 6 2	47.68
1.886	1	3 3 3	48.22
1.839	2	0 0 8	49.52
1.803	13	2 4 5	50.58
1.798	8	1 3 7	50.74
1.791	18	4 0 0	50.94
1.787	15	3 3 4	51.08
1.762	5	1 1 8	51.86
1.757	6	0 2 8	52.02
1.734	2	2 2 7	52.76
1.714	3	0 4 7 +	53.42
1.703	5	4 2 1	53.80
1.682	16	2 6 2	54.50
1.670	29	2 4 6 +	54.92
1.639	5	3 5 2	56.08
1.636	7	2 0 8	56.18
1.632	4	2 6 3	56.34
1.624	6	1 3 8	56.64
1.618	7	4 2 3	56.84
1.610	2	4 0 4	57.16
1.606	7	1 7 2	57.32
1.576	1	0 2 9	58.52
1.564	7	2 6 4 +	59.00
1.554	8	4 2 4	59.44
1.546	6	2 4 7	59.78
1.537	13	0 6 6	60.14
1.529	3	3 5 4	60.50
1.524	4	4 4 1	60.72
1.502	3	1 7 4	61.70

d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
1.500	4	4 4 2	61.80
1.481	4	4 2 5 +	62.68
1.472	3	0 8 1	63.10
1.463	3	4 4 3	63.56
1.450	3	0 8 2	64.16
1.446	7	3 1 8 +	64.36
1.443	7	2 2 9	64.54
1.431	3	1 1 10 +	65.14
1.427	2	0 2 10	65.32
1.423	3	1 5 8	65.52
1.414	4	4 4 4	66.00
1.405	1	4 2 6	66.50
1.397	2	5 1 2	66.94
1.373	1	0 8 4	68.26
1.367	5	3 3 8 +	68.60
1.361	5	2 0 10 +	68.92
1.358	3	4 4 5	69.12
1.356	3	3 7 2	69.20
1.354	2	1 3 10	69.36
1.328	4	4 2 7 +	70.88
1.326	6	4 6 0 +	71.02
1.326	6	5 3 2	71.04
1.317	3	2 8 3 +	71.56
1.305	2	4 6 2 +	72.36
1.292	2	3 7 4	73.18
1.283	1	4 0 8	73.78
1.274	2	1 9 2	74.40
1.265	1	5 3 4	75.04
1.259	3	2 6 8	75.42
1.254	2	4 2 8	75.80
1.246	1	3 1 10	76.38
1.241	2	3 5 8 +	76.74
1.238	2	4 4 7	76.96
1.231	1	1 5 10	77.46
1.226	4	0 0 12 +	77.84
1.220	1	1 9 4	78.28
1.219	1	0 4 11	78.38
1.209	2	5 5 2 +	79.14
1.1944	6	2 8 6 +	80.32
1.1786	1	6 0 2	81.62
1.1772	1	4 4 8	81.74
1.1704	2	6 2 0	82.32
1.1664	7	4 6 6 +	82.66
1.1539	1	2 4 11	83.76
1.1507	1	0 10 3	84.04
1.1384	5	2 2 12 +	85.16
1.1356	4	6 0 4	85.42
1.1328	2	0 4 12	85.68
1.1271	2	4 8 2 +	86.22
1.1240	2	2 10 0	86.52

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
7.36	26	0 0 2	12.02
5.92	11	0 2 0	14.96
5.66	3	1 1 1	15.65
5.49	95	0 2 1	16.13
4.709	90	1 1 2	18.83
4.611	43	0 2 2	19.23
3.829	3	1 1 3	23.21
3.776	55	0 2 3	23.54
3.678	6	0 0 4	24.17
3.365	2	1 3 1	26.47
3.221	73	2 0 2	27.68
3.154	71	1 1 4	28.27
3.128	46	1 3 2	28.51
3.124	57	0 2 4	28.55
3.064	100	2 2 0	29.12
3.000	39	2 2 1	29.75
2.959	10	0 4 0	30.18
2.901	17	0 4 1	30.79
2.829	1	2 2 2	31.60
2.745	12	0 4 2	32.59
2.635	16	0 2 5	33.99
2.599	12	2 2 3	34.48
2.566	22	2 0 4	34.93
2.534	15	0 4 3	35.46
2.519	12	1 3 4	35.61
2.452	4	0 0 6	36.61
2.354	1	2 2 4	38.19
2.306	26	0 4 4	39.03
2.266	4	0 2 6	39.75
2.254	7	2 4 1	39.96
2.231	4	3 1 2	40.40
2.222	3	1 5 1	40.57
2.150	20	1 5 2	41.99
2.123	8	2 2 5	42.56
2.113	1	3 1 3	42.77
2.087	6	0 4 5	43.33
2.069	12	2 4 3	43.72
2.043	2	1 5 3	44.29
2.024	1	3 3 1	44.75
2.024	1	2 0 6	44.75
1.988	2	1 1 7	45.59
1.981	10	0 2 7	45.77
1.975	24	3 1 4	45.91
1.973	7	0 6 0	45.96
1.968	5	3 3 2	46.07
1.939	2	2 4 4	46.82
1.918	4	1 5 4	47.36
1.915	15	2 2 6	47.44
1.906	3	0 6 2	47.69
1.886	1	3 3 3	48.21

d (Å)	I	hkl	$2\theta(°)$ λ = 1.54056 Å
1.839	2	0 0 8	49.52
1.803	17	2 4 5	50.58
1.796	1	1 3 7	50.80
1.791	23	4 0 0	50.95
1.786	8	3 3 4	51.10
1.762	6	1 1 8	51.86
1.756	5	0 2 8	52.02
1.733	3	2 2 7	52.77
1.716	1	2 6 1	53.33
1.714	1	4 2 0	53.40
1.714	3	0 4 7	53.42
1.703	6	4 2 1	53.79
1.682	22	2 6 2	54.50
1.670	38	2 4 6	54.92
1.670	4	4 2 2	54.95
1.639	5	3 5 2	56.07
1.636	8	2 0 8	56.17
1.630	1	2 6 3	56.41
1.624	8	1 3 8	56.64
1.618	8	4 2 3	56.85
1.610	2	4 0 4	57.16
1.606	9	1 7 2	57.32
1.576	1	0 2 9	58.52
1.564	9	2 6 4	59.01
1.562	2	0 4 8	59.09
1.554	11	4 2 4	59.44
1.546	8	2 4 7	59.77
1.537	19	0 6 6	60.15
1.529	3	3 5 4	60.50
1.524	6	4 4 1	60.72
1.502	3	1 7 4	61.69
1.500	6	4 4 2	61.80
1.481	5	4 2 5	62.67
1.480	2	0 8 0	62.74
1.472	4	0 8 1	63.10
1.463	4	4 4 3	63.56
1.451	4	0 8 2	64.15
1.446	4	4 0 6	64.36
1.446	5	3 1 8	64.36
1.442	6	2 2 9	64.55
1.431	2	0 4 9	65.13
1.431	3	1 1 10	65.15
1.428	1	0 2 10	65.29
1.423	3	1 5 8	65.52
1.417	1	0 8 3	65.88
1.414	5	4 4 4	65.99
1.405	1	4 2 6	66.49
1.397	3	5 1 2	66.95
1.373	1	0 8 4	68.27
1.368	3	2 8 0	68.56

d (Å)	I	hkl	$2\theta(°)$ λ = 1.54056 Å
1.367	7	3 3 8	68.60
1.362	3	2 8 1	68.90
1.361	4	2 0 10	68.94
1.359	2	4 4 5	69.05
1.356	3	3 7 2	69.21
1.354	2	1 3 10	69.36
1.329	1	2 4 9	70.85
1.328	4	4 2 7	70.88
1.327	3	5 1 4	70.99
1.326	4	4 6 0	71.02
1.325	4	5 3 2	71.11
1.318	1	0 4 10	71.56
1.317	3	2 8 3	71.57
1.305	2	4 6 2	72.35
1.305	1	0 2 11	72.37
1.292	3	3 7 4	73.19
1.283	1	4 0 8	73.78
1.274	3	1 9 2	74.40
1.265	1	5 3 4	75.05
1.259	5	2 6 8	75.41
1.254	3	4 2 8	75.80
1.246	1	3 1 10	76.39
1.241	3	3 5 8	76.74
1.240	1	2 8 5	76.79
1.238	2	4 4 7	76.94
1.231	2	1 5 10	77.46
1.226	4	0 0 12	77.84
1.226	2	2 2 11	77.85
1.220	2	1 9 4	78.28
1.219	1	0 4 11	78.39
1.210	1	0 8 7	79.08
1.209	3	5 5 2	79.15
1.1944	10	2 8 6	80.32
1.1940	1	3 3 10	80.35
1.1831	1	4 2 9	81.24
1.1786	2	6 0 2	81.62
1.1772	1	4 4 8	81.73
1.1704	3	6 2 0	82.31
1.1687	1	0 10 2	82.46
1.1667	2	6 2 1	82.63
1.1664	12	4 6 6	82.65
1.1539	1	2 4 11	83.75
1.1507	1	0 10 3	84.04
1.1463	1	2 8 7	84.44
1.1384	1	6 2 3	85.16
1.1384	7	2 2 12	85.16
1.1382	2	3 9 2	85.18
1.1373	2	4 8 1	85.27
1.1357	3	6 0 4	85.42
1.1328	1	0 4 12	85.69

Trimethylammonium Chloride, $(CH_3)_3NHCl$

Structure
Monoclinic, $P2_1/m$ (11), Z=2 [Lindgren and Olovsson, 1968]

Lattice parameters
a=6.088±.003, b=7.033±.002, c=7.031±.002 Å, β= 95.73°±.04° [ibid.]

Density
(calculated) 1.060 g/cm^3 [ibid.]

Thermal parameters

Isotropic:	H	6.00 [ibid.]
	Cl	5.68
	N	5.04
	C(1)	6.08
	C(2)	7.56

Scattering factors
H°, C°, N°, Cl^- [3.3.1A]

Scale factor
(integrated intensities) 0.5674×10^4

Reference
Lindgren, J. and I. Olovsson (1968). Acta Cryst. B24, 554.

Calculated Pattern *(Peak heights)*

d (Å)	*I*	*hkl*	$2\theta(^\circ)$ λ = 1.54056 Å
6.054	8	1 0 0	14.62
4.957	1	0 1 1	17.88
4.590	100	1 1 0	19.32
3.976	4	-1 1 1	22.34
3.711	1	1 1 1	23.96
3.515	15	0 2 0	25.32
3.498	41	0 0 2	25.44
3.131	3	0 1 2 +	28.48
3.042	9	1 2 0	29.34
3.029	10	2 0 0	29.46
2.906	2	1 0 2	30.74
2.890	20	-1 1 2 +	30.92
2.841	7	-1 2 1	31.46
2.781	1	2 1 0	32.16
2.740	7	1 2 1	32.66
2.685	9	1 1 2 +	33.34
2.671	6	-2 1 1	33.52
2.507	1	2 1 1	35.78
2.479	4	0 2 2	36.20
2.412	2	-2 0 2	37.24
2.354	1	-1 2 2	38.20
2.295	1	2 2 0	39.22
2.240	2	1 2 2	40.22
2.222	2	0 3 1	40.56
2.185	3	2 0 2 +	41.28
2.146	1	-1 1 3	42.08
2.108	1	-1 3 1	42.86
2.018	1	1 1 3	44.88
1.989	1	-2 2 2	45.56
1.941	2	3 1 0	46.76
1.885	1	-1 3 2	48.24
1.874	1	-2 1 3	48.54
1.854	1	2 3 0	49.10
1.825	1	3 1 1	49.92
1.820	1	-2 3 1	50.08
1.765	1	2 0 3	51.76
1.758	1	0 4 0	51.96
1.751	1	3 2 0	52.20
1.749	1	0 0 4	52.26
1.677	1	-1 1 4	54.68

Calculated Pattern *(Integrated)*			
d (Å)	I	hkl	$2\theta(°)$ $\lambda = 1.54056$ Å
6.058	7	1 0 0	14.61
4.960	1	0 1 1	17.87
4.590	100	1 1 0	19.32
3.978	4	-1 1 1	22.33
3.711	1	1 1 1	23.96
3.516	14	0 2 0	25.31
3.498	43	0 0 2	25.44
3.142	1	0 2 1	28.38
3.132	4	0 1 2	28.48
3.041	10	1 2 0	29.34
3.029	9	2 0 0	29.47
2.906	2	1 0 2	30.74
2.889	22	-1 1 2	30.92
2.887	1	-2 0 1	30.95
2.842	8	-1 2 1	31.46
2.782	1	2 1 0	32.15
2.739	8	1 2 1	32.66
2.686	7	1 1 2	33.33
2.684	5	2 0 1	33.36
2.670	6	-2 1 1	33.53
2.507	1	2 1 1	35.78
2.480	5	0 2 2	36.19
2.412	3	-2 0 2	37.25
2.354	1	-1 2 2	38.20
2.295	2	2 2 0	39.22
2.240	2	1 2 2	40.22
2.223	2	0 3 1	40.55
2.186	2	1 3 0	41.26
2.184	2	2 0 2	41.30
2.146	1	-1 1 3	42.08
2.133	1	2 2 1	42.33
2.109	2	-1 3 1	42.85
2.018	1	1 1 3	44.87
1.989	1	-2 2 2	45.57
1.941	2	3 1 0	46.77
1.897	1	-1 2 3	47.91
1.885	1	-1 3 2	48.25
1.874	1	-2 1 3	48.55
1.854	1	2 3 0	49.10
1.826	1	3 1 1	49.91
1.820	1	-2 3 1	50.08
1.771	1	-3 1 2	51.57
1.765	1	2 0 3	51.77
1.758	1	0 4 0	51.96
1.751	1	3 2 0	52.19
1.749	1	0 0 4	52.26
1.677	1	-1 1 4	54.68

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONOGRAPH 25, SECTIONS 1, 2, 3, 4, 5, 6, 8, and 9[5]

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

m–Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

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m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

m—Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

CUMULATIVE MINERAL INDEX

*Natural mineral.

M—Monagraph 25.

* Natural mineral.

m—Monograph 25.

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Section 9. ---- Data for 63 Substances

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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 63 substances. Forty of these patterns represent experimental data and 23 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 were 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

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