Standard X-Ray Diffraction Powder Patterns from The JCPDS Research Associateship

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The following new or updated patterns are submitted by the JCPDS Research Associateship at the National Bureau of Standards. The patterns are a continuation of the series of standard X-ray diffraction powder patterns published previously in the NBS Circular 539, the NBS Monograph 25, and in this journal. The methods of producing these reference patterns are described in this journal, Vol. 1, No. 1, p. 40 (1986).

The data for each phase apply to the specific sample described. A sample was mixed with one or two internal standards: silicon (SRM640a), silver, tungsten, or fluorophlogopite (SRM675). Expected 2-theta values for these standards are specified in the methods described (ibid.). Data, from which the reported 2-theta values were determined, were measured with a computer controlled diffractometer. Computer programs were used to locate peak positions and calibrate the patterns as well as to perform variable indexing and least squares cell refinement. A check on the overall internal consistency of the data was also provided by a computer program.

Intensities were measured as peak heights above background and were read manually from strip charts. To minimize orientation effects, a sample without internal standards was mixed with an amorphous material and then side mounted. Each reported intensity is the average of at least three measurements made on separate mountings of the sample.

https://doi.org/10.1017/S0885715600011829 Published online by Cambridge University Press

Bismuth Silicate, $Bi_{12}SiO_{20}$

Mineral name
Sillénite, syn

CAS registry no.
12272-31-0

Sample
The sample was made by heating Bi_2O_3 and SiO_2 in a 6:1 molar mixture up to 840°C for 16 hours.

Color
Grayish yellow

Symmetry classifications

Crystal system	Cubic
Space group	I*3*
Pearson symbol	cI66

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.9°C
2θ Standard	Silicon
σ (I^{rel})	±2

Crystallographic constants
a = 10.1067 (2) Å
V = 1032.35 Å^3
Z = 2
Density (calc.) = 9.187 g/cm^3

Figures of merit
F_{30} = 167 (0.0061, 30)
M_{20} = 191

Comment
The structure of sillénite and its relation to γ-Bi_2O_3 is discussed by Batog *et al.*[1].

Additional patterns
To replace 17-804[2] and 27-55[1].

References

1. Batog, V. N., Pakhomov, V. I., Safronov, G. M., and Fedorov, P. M. (1973). Inorg. Mater. (Engl. Transl.) *9,* 1400.
2. Gattow, G. and Fricke, H. (1963). Z. Anorg. Allg. Chem. *324,* 287.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
7.147	1	1	1	0	12.374
5.051	2	2	0	0	17.544
4.125	3	2	1	1	21.523
3.574	22	2	2	0	24.895
3.196	100	3	1	0	27.892
2.918	21	2	2	2	30.616
2.701	72	3	2	1	33.135
2.5272	3	4	0	0	35.493
2.3829	11	3	3	0	37.721
2.2607	12	4	2	0	39.844
2.1552	16	3	3	2	41.883
2.0634	9	4	2	2	43.841
1.9825	15	5	1	0	45.729
1.8454	10	5	2	1	49.344
1.7868	1L	4	4	0	51.074
1.7335	41	5	3	0	52.765
1.6846	18	6	0	0	54.421
1.6396	28	6	1	1	56.044
1.5979	1	6	2	0	57.641
1.5596	3	5	4	1	59.197
1.5238	3	6	2	2	60.731
1.4903	20	6	3	1	62.247
1.4589	2	4	4	4	63.739
1.4295	8	7	1	0	65.213
1.4014	2	6	4	0	66.688
1.3754	5	7	2	1	68.121
1.3508	3	6	4	2	69.536
1.3269	1	7	3	0	70.975
1.2835	5	6	5	1	73.760
1.2634	1	8	0	0	75.139
1.2439	3	8	1	1	76.526
1.2253	2	8	2	0	77.903
1.2080	13	6	5	3	79.233
1.1911	12	6	6	0	80.591
1.1748	12	7	5	0	81.941
1.1593	1L	6	6	2	83.277
1.1444	2	7	5	2	84.615
1.1298	1	8	4	0	85.967
1.1161	2	9	1	0	87.287
1.1029	3	8	4	2	88.606
1.0897	6	9	2	1	89.963
1.0774	1L	6	6	4	91.281
1.0654	5	9	3	0	92.607
1.0425	2	9	3	2	95.274
1.0316	1L	8	4	4	96.615
1.0210	9	7	7	0	97.959
1.0106	2	10	0	0	99.323
1.0006	1L	10	1	1	100.672
0.9910	1	10	2	0	102.030
0.9816	2	9	5	0	103.393
0.9726	1	10	2	2	104.752
0.9636	3	10	3	1	106.151
0.9466	2	3	7	1	108.937

Calcium Oxide, CaO

Mineral name
Lime, syn
Halite group, periclase subgroup

CAS registry no.
1305-78-8

Sample
The sample was prepared from $Ca(OH)_2$ obtained from Fisher Scientific Co., Fair Lawn, NJ, by heating it to 925°C overnight. It was kept under a stream of dry N_2 during data collection.

Color
Colorless

Symmetry classifications

Crystal system	Cubic
Space group	Fm3m (225)
Pearson symbol	cF8
Structure type	NaCl

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.3°C
2θ Standard	Tungsten
σ (I^{rel})	±2

Crystallographic constants
a = 4.81059 (9) Å
V = 111.33 Å^3
Z = 4
Density (calc.) = 3.346 g/cm^3

Figures of merit
F_{13} = 146 (0.0069, 13)
M_{13} = 743

Comments
The structure was determined by Oftedal[1]. References to earlier patterns will be found in reference #2.

Additional pattern
To replace PDF 4-777[2].

References

1. Oftedal, I. (1927). Z. Phys. Chem. (Leipzig) *128,* 154.
2. Swanson, H. E. and Tatge, E. (1953). Natl. Bur. Stand. (U.S.), Circ. 539 *1,* 43.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
2.777	36	1	1	1	32.204
2.4059	100	2	0	0	37.347
1.7009	54	2	2	0	53.856
1.4505	16	3	1	1	64.154
1.3888	16	2	2	2	67.375
1.2026	6	4	0	0	79.665
1.1037	6	3	3	1	88.524
1.0758	16	4	2	0	91.459
0.9819	12	4	2	2	103.343
0.9257	6	5	1	1	112.631
0.8504	6	4	4	0	129.879
0.8131	10	5	3	1	142.642
0.8018	16	6	0	0	147.776

https://doi.org/10.1017/S0885715600011829 Published online by Cambridge University Press

Calcium Sulfate, $CaSO_4$

Mineral name
Anhydrite, syn

Mineral group
Anhydrite

CAS registry no.
7778-18-9

Sample
The sample was prepared by adding an aqueous solution of K_2SO_4 to one of $CaCl_2$. The resultant precipitate was washed, dried, and then heated to 700°C for 5 hours.

Color
Colorless

Symmetry classifications

Crystal system	Orthorhombic
Space group	Bmmb (63)
Pearson symbol	oC24
Structure type	$CaSO_4$

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.8°C
2θ Standard	Silicon
σ (I^{rel})	±1

Crystallographic constants
a = 6.9933 (4) Å
b = 7.0017 (5)
c = 6.2411 (5)

a/b = 0.9988
c/b = 0.8914

V = 305.60 $Å^3$
Z = 4
Density (calc.) = 2.959 g/cm^3

Figures of merit
F_{30} = 99 (0.0066, 46)
M_{20} = 149

Comments
The definitive structure of $CaSO_4$ was determined by Höhne[1]. This form is called "insoluble anhydrite" to distinguish it from the tetragonal "soluble anhydrite" form. References to other earlier patterns will be found in reference 2.

Additional patterns
To replace PDF 6-226[2].
Bushuev *et al.*[3].

References

1. Höhne, E. (1962). Monatsber. Dtsch. Akad. Wiss. Berlin *4*, 72.
2. Swanson, H. E., Fuyat, R. K., and Ugrinic, G. M. (1955). Natl. Bur. Stand. (U.S.) Circ. 539 *4*, 65.
3. Bushuev, N. N., Masiennikov, B. M., and Borisov, V. M. (1983). Russ. J. Inorg. Chem. (Engl. Transl.) *28*, 2469.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
3.879	5	1	1	1	22.911
3.499	100	0	2	0+	25.437
3.121	2	0	0	2	28.580
2.849	29	0	1	2	31.368
2.797	3	1	2	1	31.971
2.4735	7	2	2	0	36.290
2.3282	20	2	0	2+	38.641
2.2090	20	2	1	2	40.816
2.1836	8	3	0	1	41.313
2.0865	8	1	3	1	43.331
1.9940	4	1	0	3	45.449
1.9388	3	2	2	2	46.820
1.9176	1L	1	1	3	47.370
1.8692	16	0	3	2	48.675
1.8527	3	3	2	1	49.136
1.7500	11	0	4	0	52.231
1.7481	10	4	0	0	52.290
1.7325	1L	1	2	3	52.798
1.6483	15	2	3	2	55.722
1.5944	2	3	3	1	57.778
1.5647	4	2	4	0+	58.982
1.5252	3	4	0	2	60.667
1.5158	1	1	3	3+	61.085
1.4905	5	4	1	2	62.238
1.4250	2	0	2	4+	65.443
1.4188	1	3	2	3	65.767
1.3988	3	2	4	2+	66.828
1.3961	3	2	1	4	66.975
1.3659	1L	3	4	1	68.660
1.3197	4	2	2	4	71.419
1.2971	1	0	3	4	72.865
1.2771	6	4	3	2	74.197
1.2371	1	4	4	0	77.022
1.2162	3	2	3	4	78.597
1.2000	2	2	5	2	79.867
1.1783	1	5	3	1	81.648
1.1669	4	0	6	0	82.614
1.1654	5	6	0	0	82.751
1.1640	5	4	0	4	82.869
1.1499	1	4	4	2	84.117
1.1485	1	4	1	4	84.243
1.1452	1L	5	1	3	84.541
1.1058	7	6	2	0	88.309

Cobalt Strontium Germanium Oxide, $CoSrGe_2O_6$

Sample
This sample was synthesized by F. R. Larson and G. J. McCarthy at North Dakota State Univ., Fargo, ND. Stoichiometric proportions of $SrCO_3$, Co_3O_4, and GeO_2 were mixed, calcined at 800°C for 24 hours, and at 1220°C for 72 hours with 2 intermediate grindings. This synthesis was supported by a grant from the JCPDS – International Centre for Diffraction Data.

Color
Light purple

Symmetry classifications

Crystal system	Monoclinic
Space group	I2/a (15)
Pearson symbol	mC40
Structure type	Diopside

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	24.4°C
2θ Standards	Silver, FP
σ (I^{rel})	±4

Crystallographic constants
a = 10.2439 (14) Å
b = 9.2941 (11)
c = 5.4711 (8)

β = 105.360 (13)°

a/b = 1.1022
c/b = 0.5887

V = 502.3 $Å^3$
Z = 4
Density (calc.) = 5.127 g/cm^3

Figures of merit
F_{30} = 60 (0.011, 46)
M_{20} = 44

Comments
The unit cell and space group were determined by Larson and McCarthy. Very weak peaks at two-thetas 26.15° and 38.57° could not be indexed and may be due to an impurity.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
4.645	2	0	2	0	19.093
3.832	7	-2	1	1	23.193
3.485	5	-1	2	1	25.536
3.384	21	2	2	0	26.315
3.121	100	1	2	1	28.576

(continued)

Cobalt Strontium Germanium Oxide, $CoSrGe_2O_6$ *(continued)*

d(A)	I^{rel}	h	k	ℓ	2θ (°)
3.102	22	3	1	0	28.752
3.033	24	2	1	1	29.427
2.955	4	1	3	0	30.224
2.672	31	0	3	1	33.509
2.636	75	-3	2	1+	33.982
2.469	12	4	0	0	36.352
2.419	12	-4	1	1	37.134
2.323	10	0	4	0	38.737
2.317	9	-3	1	2	38.835
2.293	5	-2	2	2+	39.259
2.257	5	-3	3	0	39.917
2.229	3	2	3	1	40.432
2.208	4	3	2	1	40.835
2.180	1L	-4	2	0	41.384
2.126	14	-1	4	1	42.488
2.106	19	2	0	2	42.913
2.101	6	-4	0	2	43.021
2.0508	6	-1	3	2	44.124
1.9908	1	4	1	1	45.527
1.9481	3	-4	3	1	46.584

d(A)	I^{rel}	h	k	ℓ	2θ (°)
1.9330	7	-5	1	0	46.970
1.9159	2	-4	2	2	47.414
1.8920	1	-3	3	2	48.051
1.8798	1	-3	4	1	48.381
1.8269	8	1	5	0	49.878
1.8005	8	3	1	2	50.660
1.7958	8	-5	1	2	50.800
1.7532	2	0	5	1	52.127
1.7419	7	-2	4	2	52.492
1.7282	8	0	1	3	52.939
1.7031	16	4	3	1	53.783
1.6922	12	4	4	0+	54.156
1.6660	3	5	3	0	55.079
1.6464	2	6	0	0	55.792
1.6284	1	-4	1	3	56.464
1.6187	10	3	5	0	56.832
1.6029	9	5	2	1+	57.446
1.5995	14	-6	0	2	57.580
1.5788	2	3	3	2	58.404
1.5663	13	-2	3	3	58.918

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
1.5485	3	0	6	0	59.662
1.5317	2	-5	4	1	60.386
1.5129	2	2	1	3+	61.215
1.4943	8	-6	3	1	62.059
1.4861	4	-1	6	1	62.442
1.4777	2	2	6	0	62.836
1.4687	17	1	5	2	63.264
1.4535	5	-5	2	3+	64.003
1.4470	3	6	1	1	64.328
1.4306	1L	-1	4	3	65.157
1.4012	1	-3	4	3	66.699
1.3954	14	7	1	0+	67.012
1.3739	5	4	5	1+	68.203
1.3678	1L	-2	0	4	68.550
1.3406	4	-3	1	4	70.144
1.3357	5	0	6	2+	70.440
1.3247	1	6	3	1	71.109

Hafnium Phosphate, HfP_2O_7

Synonym
Hafnium pyrophosphate

CAS registry no.
16726-11-7

Sample
The sample was made by stirring HfO_2 in an 85% aqueous solution of H_3PO_4 at 90°C for 24 hours.

Color
Colorless

Symmetry classifications

Crystal system	Cubic
Space group	Pa3 (205)
Pearson symbol	cP40

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	27.4°C
2θ Standards	Silicon, FP

Crystallographic constants
a = 8.1859 (2) Å
V = 548.53 Å^3
Z = 4
Density (calc.) = 4.268 g/cm^3

Figures of merit
F_{30} = 124 (0.0075, 32)
M_{20} = 152

Comments
The structure of HfP_2O_7 is isostructural with ZrP_2O_7, the structure of which was determined by Levi and Peyronel[1]. At higher temperatures HfP_2O_7 transforms to a cell with a tripled 'a' dimension[2].

Additional pattern
To replace PDF 3-1141[1].

References

1. Levi, G. R. and Peyronel, G. (1935). Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem. *92*, 190.
2. Vollenkle, H., Wittmann, A., and Nowotny, H. (1963). Monatsh. Chem. *94*, 956.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
4.726	47	1	1	1	18.763
4.093	100	2	0	0	21.695
3.661	19	2	1	0	24.293
3.344	17	2	1	1	26.633
2.894	44	2	2	0	30.875
2.730	2	2	2	1	32.780
2.468	64	3	1	1	36.373
2.363	12	2	2	2	38.051
2.270	3	2	3	0	39.666
2.1881	1L	3	2	1	41.225
2.0466	7	4	0	0	44.220
1.9861	3	3	2	2	45.640
1.9298	2	4	1	1	47.052
1.8779	22	3	3	1	48.434
1.3804	29	4	2	0	49.775

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
1.7862	2	4	2	1	51.094
1.7458	2	3	3	2	52.366
1.6709	20	4	2	2	54.904
1.6377	2	4	3	0	56.115
1.5753	29	5	1	1	58.549
1.5197	1L	2	5	0	60.912
1.4947	1L	5	2	1	62.041
1.4471	8	4	4	0	64.322
1.4249	1L	5	2	2	65.451
1.4042	1L	4	3	3	66.540
1.3836	13	5	3	1	67.660
1.3642	9	6	0	0	68.755
1.3283	1	6	1	1	70.887
1.2944	5	6	2	0	73.038
1.2733	1L	4	5	0	74.110
1.2484	5	5	3	3	76.200
1.2338	4	6	2	2	77.269
1.2204	1L	6	3	0	78.276
1.2067	1L	6	3	1	79.340
1.1815	1L	4	4	4	81.378
1.1694	4	6	3	2	82.400
1.1574	1L	5	4	3	83.450
1.1464	4	5	5	1	84.434
1.1351	5	6	4	0	85.467
1.1243	1L	6	4	1	86.493
1.1139	1L	7	2	1	87.500
1.0940	5	6	4	2	89.517
1.0658	8	7	3	1	92.560
1.0479	1	6	4	3	94.630
1.0231	1	8	0	0	97.690
1.0000	3	7	3	3	100.760
0.9927	4	6	4	4	101.781
0.9647	3	6	6	0	105.975
0.9435	4	7	5	1	109.156
0.8985	3	9	1	1	118.030
0.8932	2	8	4	2	119.170
0.8727	2	6	6	4	123.929
0.8580	4	9	3	1	127.732

https://doi.org/10.1017/S0885715600011829 Published online by Cambridge University Press

Iron Lanthanum Oxide, $FeLaO_3$

Synonym
Lanthanum orthoferrite

CAS registry no.
12022-43-4

Sample
Stoichiometric amounts of $La(OH)_3$ and Fe_2O_3 were mixed and heated overnight at 1000°C, then 1 day each at 1200°C and 1350°C with intermediate regrindings.

Color
Dark brown

Symmetry classifications

Crystal system	Orthorhombic
Space group	Pn*a
Pearson symbol	oP20
Structure type	Distorted perovskite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.4°C
2θ Standard	Tungsten
σ (I^{rel})	±3

Crystallographic constants
a = 5.5669 (4) Å
b = 7.8547 (7)
c = 5.5530 (8)

a/b = 0.7087
c/b = 0.7070

V = 242.81 Å^3
Z = 4
Density (calc.) = 6.640 g/cm^3

Figures of merit
F_{30} = 34 (0.011, 84)
M_{20} = 50

Comments
The structure was determined qualitatively by Geller and Wood[1]. A rhombohedral phase was found above 980°C (Dalziel[2]).

Additional pattern
To replace PDF 15-148[1].

References

1. Geller, S. and Wood, E. A. (1956). Acta Crystallogr. *9,* 563.
2. Dalziel, J. A. W. (1959). J. Chem. Soc. *1959,* 1993.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
3.930	17	1	0	1+	22.606
3.517	4	1	1	1	25.304
2.779	100	1	2	1+	32.190
2.624	3	2	1	0	34.145
2.487	1L	2	0	1	36.090
2.370	3	1	1	2+	37.938
2.270	18	2	2	0	39.674
2.180	3	1	3	1	41.389
2.1018	1L	2	2	1	43.000
1.9656	30	2	0	2	46.144
1.9074	5	2	3	0+	47.638
1.8027	1	1	3	2	50.592
1.7572	7	1	4	1+	51.999
1.7173	4	3	1	1	53.303
1.6041	39	2	4	0+	57.399
1.5722	1	2	3	2	58.676
1.5419	1L	2	4	1+	59.945
1.5113	1L	0	3	3+	61.288
1.4605	3	3	3	1	63.661
1.3892	15	2	4	2	67.349
1.3705	2	4	1	0	68.398
1.3676	1L	2	5	0	68.563
1.3293	1L	3	3	2	70.825
1.3278	1L	1	5	2+	70.920
1.3094	4	1	4	3+	.72.068
1.2923	1	3	1	3	73.177
1.2423	1l	2	0	4+	76.641
1.2288	2	4	1	2+	77.638
1.2276	2	2	5	2	77.732
1.1976	1L	0	5	3+	80.065
1.1847	3	2	6	0+	81.116
1.1721	2	3	5	1+	82.169
1.1355	4	4	4	0	85.434
1.1336	3	0	4	4	85.614
1.1237	1	4	3	2	86.553
1.1013	1L	4	1	3	88.766
1.1003	1L	2	5	3	88.866
1.0896	2	2	6	2	89.978
1.0813	1	5	1	1	90.853
1.0788	1	1	1	5+	91.133
1.0499	13	2	4	4	94.389
1.0419	1L	4	5	0	95.349
1.0232	1L	3	3	4	97.670
1.0075	1	5	3	1	99.737
1.0063	1	3	5	3	99.904
0.9829	2	4	0	4	103.198
0.9819	1	0	8	0	103.353
0.9754	2	4	5	2+	104.319
0.9537	2	4	6	0	107.745
0.9526	1	1	8	1	107.921
0.9471	1	5	1	3	108.841
0.9459	1L	3	1	5+	109.049
0.9272	4	5	2	3	112.354
0.9262	9	3	6	3+	112.543

Molybdenum Sulfide, MoS_2

Mineral name
Molybdenite, 2H, syn

Mineral group
Molydenite group

CAS registry no.
1317-33-5

Sample
The sample was obtained from Aesar, Seabrook, NH, a branch of Johnson Matthey. It was labeled 98% MoS_2.

Color
Very dark gray

Symmetry classifications

Crystal system	Hexagonal
Space group	$P6_3/mmc$ (194)
Pearson symbol	hP6

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.8°C
2θ Standard	Silver
σ (I^{rel})	±4

Crystallographic constants
a = 3.16116 (12) Å
c = 12.2985 (5)

c/a = 3.8905

V = 106.43 Å^3
Z = 2
Density (calc.) = 4.994 g/cm^3

Figures of merit
F_{30} = 70 (0.011, 39)
M_{20} = 105

Comments
The structure was determined by Dickinson and Pauling[1]. A rhombohedral form of molybdenite, with 'c' multiplied by 1.5, was found as a natural mineral (Traill[2]). References to other early patterns will be found in reference 3.

Additional pattern
To replace PDF 6-97, Swanson *et al.*[3].

References

1. Dickinson, R. G. and Pauling, L. G. (1923). J. Am. Chem. Soc. *45,* 1466.
2. Traill, J. (1963). Can. Mineral. *7,* 524.
3. Swanson, H. E., Gilfrich, N. T., and Ugrinic, G. M. (1955). Natl. Bur. Stand. (U.S.) Circ. 539 *5,* 47.

(continued)

Molybdenum Sulfide, MoS_2 *(continued)*

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
6.155	100	0	0	2	14.378
3.074	2	0	0	4	29.027
2.738	22	1	0	0	32.677
2.672	12	1	0	1	33.509
2.501	10	1	0	2	35.871
2.277	58	1	0	3	39.539
2.0496	11	0	0	6	44.152
1.8299	29	1	0	5	49.788
1.6414	4	1	0	6	55.978
1.5805	14	1	1	0	58.336
1.5372	12	0	0	8	60.146
1.4782	2	1	0	7	62.815
1.4055	1L	1	1	4	66.468
1.3691	3	2	0	0	68.476
1.3601	2	2	0	1	68.995
1.3406	5	1	0	8	70.144
1.2982	7	2	0	3	72.790
1.2514	7	1	1	6	75.982
1.2297	2	0	0	10	77.572
1.2225	2	1	0	9	78.119
1.1961	4	2	0	5	80.182
1.1384	1	2	0	6	85.169
1.1220	1L	1	0	10	86.714
1.1018	10	1	1	8	88.712
1.0799	1L	2	0	7	91.009
1.0350	9	1	0	11	96.186
1.0222	3	2	0	8	97.808
1.0032	6	2	1	3	100.320
0.9707	2	1	1	10	105.039
0.9670	1	2	0	9	105.616
0.9537	5	2	1	5	107.738
0.9125	3	3	0	0	115.155
0.9026	1	3	0	2	117.165
0.8941	5	1	0	13	118.969
0.8908	1	3	0	3	119.702
0.8785	1	0	0	14	122.534
0.8658	4	2	0	11	125.674
0.8584	2	2	1	8	127.636
0.8365	1	1	0	14	134.102
0.8337	1	3	0	6	135.011

Potassium Cyanide, KCN

CAS registry no.
151-50-8

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

Color
Colorless

Symmetry classifications

Crystal system	Cubic
Space group	Fm3m (225)
Pearson symbol	cF12
Structure type	NaCl

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.5°C
2θ Standard	Silver
σ (I^{rel})	±2

Crystallographic constants
a = 6.5271 (3) Å

V = 278.07 $Å^3$
Z = 4
Density (calc.) = 1.555 g/cm^3

Figures of merit
F_{16} = 124 (0.0081, 16)
M_{16} = 329

Comments
Cooper[1,2] and Pauling[3] studied the structure. KCN has the NaCl structure with a disordered CN group. Two polymorphic forms have been reported: monoclinic (Parry[4]) and orthorhombic (Bijvoet and Lely[5]). References to other patterns may be found in reference 6.

Additional pattern
To replace PDF 4-547[6].

References

1. Cooper, P. A. (1921). Nature *107,* 745.
2. Cooper, P. A. (1922). Nature *110,* 544.
3. Pauling, L. (1930). Phys. Rev. *36,* 430.
4. Parry, G. S. (1962). Acta Crystallogr. *15,* 601.
5. Bijvoet, J. M. and Lely, J. A. (1940). Recl. Trav. Chim. Pays-Bas *59,* 908.
6. Swanson, H. E. and Tatge, E. (1953). Natl. Bur. Stand. (U.S.), Circ. 539 *1,* 77.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
3.770	19	1	1	1	23.581
3.266	100	2	0	0	27.287
2.3078	47	2	2	0	38.997
1.9684	13	3	1	1	46.074
1.8845	10	2	2	2	48.253
1.6318	3	4	0	0	56.336
1.4975	5	3	3	1	61.913
1.4595	7	4	2	0	63.713
1.3323	4	4	2	2	70.646
1.2560	2	5	1	1	75.654
1.1537	1L	4	4	0	83.774
1.1033	2	5	3	1	88.558
1.0877	1	6	0	0	90.173
1.0322	1L	6	2	0	96.535
0.9954	1	5	3	3	101.407
0.9839	1L	6	2	2	103.051

Sodium Cyanide, NaCN

CAS registry no.
143-33-9

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

Color
Colorless

Symmetry classifications

Crystal system	Cubic
Space group	Fm3m (225)
Pearson symbol	cF12
Structure type	NaCl

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	24.4°C
2θ Standard	Tungsten
σ (I^{rel})	±1

Crystallographic constants
a = 5.8894 (4) Å

V = 204.27 $Å^3$
Z = 4
Density (calc.) = 1.594 g/cm^3

Figures of merit
F_{10} = 119 (0.0084, 10)
M_{10} = 397

Comments
Verweel and Bijvoet[1] studied the structure of NaCN. Verweel and Bijvoet[2] reported a low temperature orthorhombic form. Siegel[3] reported a rhombohedral form produced by quenching the cubic form from 300°C. The cubic and rhombohedral forms coexist between 20°C and 80°C. References to other patterns are given in reference 4.

Additional pattern
To replace PDF 4-665[4]. *(continued)*

https://doi.org/10.1017/S0885715600011829 Published online by Cambridge University Press

Sodium Cyanide, NaCN *(continued)*

References

1. Verweel, H. J. and Bijvoet, J. M. (1933). Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem. *100,* 201.
2. Verweel, H. J. and Bijvoet, J. M. (1935) Recl. Trav. Chim. Pays-Bas *54,* 631.
3. Siegel, L. A. (1949). J. Chem. Phys. *17,* 1146.
4. Swanson, H. E. and Tatge, E. (1953). Natl. Bur. Stand. (U.S.), Circ. 539 *1,* 78.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
3.402	1L	1	1	1	26.176
2.945	100	2	0	0	30.328
2.0826	30	2	2	0	43.415
1.7761	4	3	1	1	51.405
1.6996	5	2	2	2	53.902
1.4726	2	4	0	0	63.080
1.3511	1	3	3	1	69.519
1.3168	2	4	2	0	71.605
1.2021	1L	4	2	2	79.705
1.1334	1L	5	1	1	85.627

Sodium Lead Phosphate, $Na_4Pb(PO_3)_6$

Sample

The sample was made by heating a 2:1:6 molar mixture of Na_2CO_3, $PbCO_3$, and $(NH_4)_2HPO_4$ at 200°C for 44 hours, at 400°C for 2 hours, and at 500°C for 110 hours with intermittent grinding.

Color

Colorless

Symmetry classifications

Crystal system	Anorthic
Space group	$P\bar{1}$ (2)
Pearson symbol	aP29

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Approx. temperature	26°C
2θ Standards	Silver, FP
$\sigma(I^{rel})$	±4

Crystallographic constants

a = 7.8072 (12) Å
b = 7.8390 (12)
c = 7.2550 (12)
α = 102.059 (14)°
β = 95.472 (13)
γ = 117.316 (13)

a/b = 0.9959
c/b = 0.9255

V = 376.33 Å^3
Z = 1
Density (calc.) = 3.411 g/cm^3

Figures of merit

F_{30} = 99 (0.0080, 38)
M_{20} = 41

Comment

Isomorphous with $Na_4Ba(PO_3)_6$, the structure of which was determined by Averbuch-Pouchot and Durif[1].

Reference

1. Averbuch-Pouchot, M. T. and Durif. A. (1983). Z. Kristallogr. *164,* 307.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
6.928	32	0	0	1	12.767
6.779	38	1	0	0	13.050
6.679	38	0	1	0+	13.246
5.686	11	0	-1	1	15.572
5.480	13	-1	0	1	16.162
4.971	2	1	-1	1	17.830
4.645	7	-1	1	1	19.091
4.380	49	1	0	1	20.256
4.234	29	0	1	1	20.964
3.916	2	-1	-1	1	22.690
3.889	1	1	1	0+	22.850
3.836	5	-1	2	0	23.170
3.688	71	1	-2	1	24.114
3.520	29	-2	1	1	25.280
3.510	38	0	-1	2	25.352
3.412	34	0	-2	1	26.092
3.400	34	-1	0	2	26.190
3.384	27	2	0	0	26.316
3.331	10	-2	2	0	26.740
3.270	28	2	-1	1	27.251
3.161	74	1	-1	2	28.209
3.071	85	-1	-1	2	29.049
3.033	71	1	1	1	29.429
2.990	5	-1	1	2	29.861
2.927	100	-2	2	1	30.520
2.876	2	1	-2	2	31.068
2.837	8	1	0	2	31.505
2.805	2	2	0	1	31.880
2.766	14	0	1	2	32.336
2.740	32	-2	0	2	32.660
2.718	32	0	2	1	32.924
2.643	29	-2	-1	1	33.885
2.569	53	1	-3	1	34.900
2.552	61	-3	1	0+	35.138
2.537	33	-3	2	0+	35.358
2.487	5	2	-2	2	36.090
2.358	21	3	-2	1	38.140
2.348	23	-1	0	3	38.310
2.320	39	0	-3	1	38.779
2.3141	25	1	-3	2	38.886
2.3070	22	0	0	3	39.010
2.2991	23	-3	0	1	39.151
2.2916	14	3	-1	1	39.283
2.2761	5	1	1	2	39.562
2.2479	3	-2	3	1	40.080
2.2217	35	-3	3	0	40.574
2.2158	25	0	-2	3	40.685
2.2059	9	-3	1	2+	40.876
2.1905	9	2	0	2	41.178
2.1819	8	1	-2	3+	41.347
2.1587	7	3	-3	1	41.811
2.1364	13	-1	1	3+	42.270
2.1175	11	0	2	2	42.664
2.0745	10	-3	3	1+	43.594
2.0628	18	-2	1	3	43.855
2.0502	11	1	0	3	44.138
2.0340	19	-2	-2	1	44.507
2.0095	10	-2	-1	3+	45.079
1.9479	12	-1	-3	1+	46.589
1.9433	11	-3	-1	1+	46.704
1.9308	14	3	-3	2	47.026
1.9127	5	2	-1	3	47.493
1.8940	13	-2	3	2+	47.997
1.8882	14	-4	1	1	48.152
1.8746	4	-4	1	0+	48.525
1.8517	16	2	-3	3	49.164
1.8437	30	-3	1	3+	49.391
1.8329	10	-1	3	2	49.703
1.8283	5	2	1	2	49.835

https://doi.org/10.1017/S0885715600011829 Published online by Cambridge University Press

Sodium Sulfite, Na_2SO_3

Synonym
Disodium sulfite

CAS registry no.
7757-83-7

Sample
The sample was obtained from the Mallinckrodt Chemical Co., St. Louis, MO.

Color
Colorless

Symmetry classifications

Crystal system	Hexagonal
Space group	$P\bar{3}$ (147)
Pearson symbol	hP12

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.7°C
2θ Standards	Silicon, FP
σ (I^{rel})	±2

Crystallographic constants
a = 5.4593 (2) Å
c = 6.1655 (2)

c/a = 1.1294

V = 159.14 $Å^3$
Z = 2
Density (calc.) = 2.630 g/cm^3

Figures of merit
F_{30} = 67 (0.012, 38)
M_{20} = 105

Comments
The structure of Na_2SO_3 was determined by Zachariasen and Buckley[2] and confirmed by Larsson and Kierkegaard[3]. Other patterns and references are cited in reference 1.

Additional pattern
To replace PDF 5-653[1].

References

1. Swanson, H. E., Fuyat, R. K., and Ugrinic, G. M. (1954). Natl. Bur. Stand. (U.S.) Circ. 539 *3,* 60.
2. Zachariasen, W. H. and Buckley, H. E. (1931). Phys. Rev. *37,* 1295.
3. Larsson, L. O. and Kierkegaard, P. (1969). Acta Chem. Scand. *23,* 2253.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
4.732	3	1	0	0	18.737
3.753	66	1	0	1	23.689
3.084	28	0	0	2	28.929
2.731	79	1	1	0	32.768
2.583	100	1	0	2	34.696
2.495	18	1	1	1	35.962
2.364	5	2	0	0	38.027
2.208	13	2	0	1	40.840
2.056	1	0	0	3	44.013
2.045	2	1	1	2	44.261
1.8764	54	2	0	2	48.475
1.7867	5	2	1	0	51.078
1.7163	2	2	1	1	53.334
1.6417	4	1	1	3	55.964
1.5761	18	3	0	0	58.515
1.5461	30	2	1	2	59.765
1.5418	2	0	0	4	59.950
1.5267	1	3	0	1	60.605
1.4658	11	1	0	4	63.407
1.3650	12	2	2	0	68.712
1.3489	1	2	1	3	69.649
1.3425	1L	1	1	4	70.029
1.3110	1L	3	1	0	71.969
1.2912	8	2	0	4	73.248
1.2829	4	3	1	1	73.802
1.2509	1	3	0	3	76.022
1.2067	12	3	1	2	79.342
1.1817	1L	4	0	0	81.365
1.1672	13	2	1	4	82.592
1.1608	1L	4	0	1	83.152
1.1238	1L	1	1	5	86.537
1.1037	6	4	0	2	88.517
1.0931	1	2	0	5	89.605
1.0684	2	3	2	1	92.274
1.0318	7	4	1	0	96.589
1.0275	1	0	0	6	97.123
1.0231	8	3	2	2	97.689
1.0176	1	4	1	1	98.391
1.0147	1L	2	1	5	98.774
0.9989	5	3	1	4	100.918
0.9784	1L	4	1	2	103.871
0.9616	6	1	1	6	106.453
0.9592	1	3	2	3	106.854
0.9379	2	4	0	4	110.422
0.9221	1	4	1	3	113.303
0.9100	2	3	3	0	115.663
0.9039	3	5	0	2	116.902
0.8909	1L	2	1	6	119.691
0.8870	3	3	2	4	120.565
0.8842	1L	4	2	1	121.188
0.8659	1L	1	0	7	125.649
0.8607	4	3	0	6	127.002
0.8582	6	4	2	2	127.672
0.8320	1L	3	3	3	135.598
0.8254	1L	2	0	7	137.906
0.8209	3	2	2	6	139.557
0.8186	6	5	1	2	140.434
0.8060	2	5	0	4	145.766

Terbium Fluoride, TbF_3

CAS registry no.
13708-63-9

Sample
The sample was obtained from the Michigan Chemical Corp., Saint Louis, MI.

Color
Yellowish white

Symmetry classifications

Crystal system	Orthorhombic
Space group	Pnma (62)
Pearson symbol	oP16

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	26.1°C
2θ Standard	Silver
σ (I^{rel})	±2

Crystallographic constants
a = 6.5082 (4) Å
b = 6.9479 (4)
c = 4.3908 (3)

a/b = 0.9367
c/b = 0.6320

V = 198.54 $Å^3$
Z = 4
Density (calc.) = 7.223 g/cm^3

Figures of merit
F_{30} = 165 (0.0047, 39)
M_{20} = 185

Comments
This phase is isostructural with YF_3, the structure of which was determined by Zalkin and Templeton[1]. Thoma and Brunton[2] reported a hexagonal phase. The transition temperature is 950°C.

Additional pattern
PDF 32-1290 (integrated intensities)[3].

References

1. Zalkin, A. and Templeton, D. H. (1953). J. Am. Chem. Soc. *75,* 2543.
2. Thoma, R. E. and Brunton, C. D. (1966). Inorg. Chem. *11,* 1937.
3. Greis, O. (1976). Ph.D. Thesis, Univ. Freiburg i. Br., Germany.

(continued)

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Terbium Fluoride, TbF_3 *(continued)*

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
3.713	34	0	1	1	23.949
3.641	66	1	0	1	24.430
3.475	72	0	2	0	25.612
3.225	100	1	1	1	27.637
2.947	72	2	1	0	30.308
2.614	5	2	0	1	34.278
2.5131	23	1	2	1	35.699
2.4469	3	2	1	1	36.699
2.3744	3	2	2	0	37.861
2.1955	14	0	0	2	41.080
2.0890	21	2	2	1	43.276
2.0483	2	0	3	1	44.180
1.9925	28	1	1	2	45.486
1.9539	58	1	3	1	46.436
1.9446	52	3	0	1	46.671
1.8870	41	2	3	0	48.186
1.8728	23	3	1	1	48.573
1.8558	16	0	2	2	49.048
1.7845	18	1	2	2	51.145
1.7605	20	2	1	2	51.896

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
1.7370	13	0	4	0	52.652
1.6972	19	3	2	1	53.983
1.6270	8	4	0	0	56.515
1.5674	7	1	4	1	58.873
1.5475	5	1	3	2	59.707
1.5429	6	3	0	2	59.903
1.5064	7	3	1	2	61.508
1.4899	13	4	1	1+	62.262
1.4734	7	4	2	0	63.041
1.4466	4	2	4	1	64.347
1.4311	15	2	3	2	65.131
1.4276	9	1	0	3	65.307
1.4102	4	3	2	2	66.216
1.3989	3	1	1	3	66.822
1.3971	2	4	2	1	66.919
1.3619	5	0	4	2	68.889
1.3347	9	2	0	3	70.501
1.3312	6	4	3	0	70.714
1.3251	2	0	5	1	71.084
1.3209	2	1	2	3	71.347

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
1.3108	2	2	1	3	71.982
1.3069	4	4	0	2	72.229
1.2981	10	1	5	1	72.795
1.2954	10	3	4	1	72.974
1.2780	4	2	5	0	74.130
1.2744	4	4	3	1	74.376
1.2462	10	2	2	3	76.357
1.2372	2	0	3	3	77.017
1.2272	6	2	5	1	77.760
1.2232	7	4	2	2	78.060
1.2133	1	3	0	3	78.821
1.1953	1	3	1	3	80.250
1.1876	3	4	4	0	80.874
1.1745	3	5	2	1	81.972
1.1579	5	0	6	0	83.404
1.1565	5	2	3	3	83.530
1.1456	1	3	2	3	84.506
1.1305	2	3	5	1	85.900
1.1197	2	5	0	2	86.935

Zinc Borate, $Zn_3B_2O_6$

CAS registry no.
1332-07-6

Sample
The sample was made by heating a 3:2 molar mixture of ZnO and H_3BO_3 up to 1000°C for 2 days with a grinding after 1 day.

Color
Colorless

Symmetry classifications

Crystal system	Monoclinic
Space group	Ia (9)
Pearson symbol	mC88

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.9°C
2θ Standard	Silicon
σ (I^{rel})	±3

Crystallographic constants
a = 23.430 (3) Å
b = 5.0457 (7)
c = 8.3848 (9)
β = 97.492 (10)°
a/b = 4.6436
c/b = 1.6618
V = 982.80 $Å^3$
Z = 8
Density (calc.) = 4.241 g/cm^3

Figures of merit
F_{30} = 115 (0.0067, 39)
M_{20} = 64

Comments
The structure of $Zn_3B_2O_6$ has been determined by Garcia-Blanco and Fayos[1]. Another form of $Zn_3B_2O_6$ stable above 964°C has been reported[2]. The formula $Zn_5B_4O_{11}$ was earlier applied to this phase[4].

Additional patterns
To replace PDF 22-1005[5], 9-116[2], and 19-1455[6]
PDF 27-983 (calculated), Bauer[3]

References

1. Garcia-Blanco, S. and Fayos, J. (1968). Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem., *127,* 145.
2. Harrison, D. E. and Hummel, F. A. (1956). J. Electrochem. Soc. *103,* 491.
3. Bauer, H. (1963). Z. Anorg. Allg. Chem. *320,* 306.
4. Whitaker, A. (1972). J. Mater. Sci. *7,* 189.
5. Gotz, W., Herrmann, V., and Ihl, R. (1969). Z. Anorg. Allg. Chem. *367,* 281.
6. Petzoldt, J. (1966). Glastech. Ber. *39,* 130.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
11.60	1	2	0	0	7.615
5.806	2	4	0	0	15.247
4.229	25	-3	1	0	20.992
4.157	25	0	0	2	21.360
4.135	30	-2	1	1	21.471
4.089	9	-2	0	2	21.719
3.954	1L	2	1	1	22.470
3.873	2	6	0	0	22.945
3.762	1	2	0	2	23.630
3.612	11	-4	0	2	24.630
3.579	15	-4	1	1	24.855
3.418	13	-5	1	0	26.050
3.355	73	4	1	1	26.544
3.225	32	-1	1	2	27.640
3.188	100	4	0	2	27.964

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
3.076	10	-3	1	2	29.006
3.038	16	-6	0	2	29.380
2.984	25	-6	1	1	29.924
2.905	26	8	0	0	30.757
2.864	4	3	1	2	31.206
2.789	38	6	1	1	32.071
2.774	27	-5	1	2+	32.248
2.666	5	6	0	2	33.591
2.541	41	-8	0	2	35.287
2.523	46	0	2	0+	35.561
2.488	44	-8	1	1	36.070
2.433	37	-7	1	2+	36.920
2.428	35	0	1	3	36.997
2.3922	20	1	2	1	37.569
2.3377	32	-4	1	3	38.478
2.3304	34	-3	2	1	38.603
2.2972	14	-9	1	0	39.184
2.2467	7	8	0	2	40.102
2.1984	12	7	1	2	41.022
2.1757	5	-5	2	1	41.470
2.1504	21	-10	0	2	41.980
2.1465	17	-2	2	2	42.060
2.1101	9	5	2	1	42.821
2.0937	13	-2	0	4	43.173
2.0684	2	-4	2	2	43.730
2.0426	1	-4	0	4	44.310
1.9998	18	2	0	4	45.311
1.9896	23	10	1	1	45.557
1.9786	25	4	2	2+	45.823
1.9590	3	6	1	3	46.310
1.9414	37	-6	2	2	46.754
1.9361	45	12	0	0	46.888
1.9187	3	9	1	2+	47.340
1.8968	2	1	1	4	47.920
1.8810	2	4	0	4	48.350
1.8526	6	-11	1	2	49.138
1.8465	6	1	2	3	49.311
1.8145	1	3	1	4	50.240
1.8048	3	-8	0	4	50.530
1.7985	4	-9	2	1	50.720
1.7902	5	-8	2	2	50.972
1.7662	18	8	1	3	51.714

https://doi.org/10.1017/S0885715600011829 Published online by Cambridge University Press

Zinc Silicate, Zn_2SiO_4

Mineral name
Willemite, syn

Mineral group
Phenakite group

Synonym
Zinc orthosilicate

CAS registry no.
13597-65-4

Sample
The sample was prepared by heating a 2:1 molar mixture of ZnO and SiO_2 (gel) up to 1300°C for 3 days.

Color
Colorless

Symmetry classifications

Crystal system	Rhombohedral
Space group	$R\bar{3}$ (148)
Pearson symbol	hR42
Structure type	Phenakite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Approx. temperature	26°C
2θ Standards	Silver, FP
σ (I^{rel})	±2

Crystallographic constants
(Hexagonal axes)
a = 13.9381 (4) Å
c = 9.3100 (4)

c/a = 0.6680

V = 1566.35 Å^3
Z = 18
Density (calc.) = 4.252 g/cm^3

Figures of merit
F_{30} = 181 (0.0042, 39)
M_{20} = 158

Comments
The structure was determined by Gottfried[1]. Rooksby and McKeag[2] report a high temperature triclinic phase. Syono *et al.*[3] and Marumo and Syono[4] report 4 other phases. References to earlier patterns may be found in reference 5.

Additional pattern
To replace PDF 8-492[5].

References

1. Gottfried, C. (1927). Neues Jahrb. Mineral., Geol. Palaeontol., Abh., Abt. A. *55A,* 393.
2. Rooksby, H. P. and McKeag, A. H. (1941). Trans. Faraday Soc. *37,* 308.
3. Syono, Y., Akinoto, S., and Matsui, Y. (1971). J. Solid State Chem. *3,* 369.
4. Marumo, F. and Syono, Y. (1971). Acta Crystallogr., Sect. B. *27,* 1968.
5. Swanson, H. E., Gilfrich, N. T., and Cook, M. I. (1957). Natl. Bur. Stand. (U.S.) Circ. 539 *7,* 62.

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
7.380	5	1	0	1	11.982
6.973	14	1	1	0	12.684
5.063	1	0	2	1	17.503
4.343	3	0	1	2	20.435
4.097	16	2	1	1	21.672
4.024	33	3	0	0	22.072
3.686	1L	2	0	2	24.123
3.485	72	2	2	0	25.542
3.258	4	1	2	2	27.352
3.151	6	1	3	1	28.300
2.8350	100	1	1	3	31.532
2.7179	1	3	1	2	32.928
2.6344	36	4	1	0	34.004
2.5325	2	0	4	2	35.416
2.3799	2	2	3	2	37.770
2.3174	50	2	2	3	38.828
2.2859	4	1	0	4	39.385
2.2159	2	2	4	1	40.685
2.1431	6	5	0	2	42.130
2.1111	1L	5	1	1	42.800
2.0730	3	2	1	4	43.626
2.0479	5	4	2	2	44.190
2.0121	10	6	0	0	45.019
2.0087	7	4	1	3	45.100
1.9653	3	1	5	2	46.152
1.9408	3	4	3	1	46.770
1.9328	11	5	2	0	46.973
1.9109	1L	1	3	4	47.545
1.8597	40	3	3	3	48.939
1.8253	2	3	4	2	49.923
1.8060	2	1	6	1	50.494
1.7795	1L	2	0	5	51.300
1.7237	2	1	2	5	53.088
1.6958	1	7	0	1	54.033
1.6883	9	6	0	3	54.292
1.6755	2	0	5	4	54.740
1.6475	4	6	2	1	55.750
1.6406	8	5	2	3	56.006
1.6290	2	2	4	4	56.440
1.6274	1	3	1	5	56.500
1.6168	2	0	7	2	56.906
1.5989	14	7	1	0	57.600
1.5864	1	5	1	4	58.098
1.5517	17	0	0	6	59.528
1.5206	9	6	3	0	60.871
1.5144	6	1	1	6	61.150
1.4669	1L	4	5	2	63.352
1.4564	1	2	7	1	63.864
1.4478	2	3	0	6	64.290
1.4428	1L	4	2	5	64.540
1.4213	34	7	1	3	65.636
1.4176	24	2	2	6	65.827
1.3938	5	5	5	0	67.101
1.3855	1	7	0	4	67.555
1.3656	18	6	3	3	68.676
1.3578	1L	3	4	5	69.128
1.3412	5	9	0	0	70.104
1.3368	19	4	1	6	70.373
1.3271	1L	6	4	2	70.960
1.3170	1	8	2	0	71.593

https://doi.org/10.1017/S0885715600011829 Published online by Cambridge University Press

Zirconium Oxide, ZrO_2

Mineral name
Baddeleyite, syn

Synonym
Zirconium dioxide

CAS registry no.
1314-23-4

Sample
The sample was obtained from the Titanium Alloy Manufacturing Co. (1960) and was heated to 1300°C for 48 hours.

Spectrographic analysis
Spectrographic analysis at NBS showed that the sample contained less than 0.01% each of Al, Hf, and Mg and between 0.1 and 0.01% each of Fe, Si, and Ti.

Color
Colorless

Symmetry classifications

Crystal system	Monoclinic
Space group	$P2_1/a$ (14)
Pearson symbol	mP12

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Scanned to	5° 2θ
Wavelength	1.5405981 Å
Mean temperature	25.5°C
2θ Standards	Silver, FP
σ (I^{rel})	±1

Crystallographic constants
a = 5.3129 (5) Å
b = 5.2125 (4)
c = 5.1471 (5)
β = 99.218 (8)°
a/b = 1.0193
c/b = 0.9875
V = 140.70 $Å^3$
Z = 4
Density (calc.) = 5.817 g/cm^3

Figures of merit
F_{30} = 101 (0.0076, 39)
M_{20} = 99

Comments
The structure of ZrO_2 (baddeleyite) was determined by McCullough and Trueblood[1] and confirmed by Smith and Newkirk[2]. There are a number of polymorphic forms of ZrO_2 stable at different temperatures and pressures[3].

Additional pattern
To replace 13-0307[4].

References

1. McCullough, J. D. and Trueblood, K. N. (1959). Acta Crystallogr. *12,* 507.
2. Smith, D. K. and Newkirk, H. W. (1965). Acta Crystallogr. *18,* 983.
3. Levin, E. M. and McMurdie, H. F. (1975). *Phase Diagrams for Ceramists, (1975) Supplement.* (American Ceramic Society, Columbus, OH), 76.
4. Lewis, General Electric Co., Cincinnati, OH. (private communication)

d(Å)	I^{rel}	h	k	ℓ	2θ (°)
5.087	3	0	0	1	17.419
3.698	14	1	1	0	24.048
3.639	10	0	1	1	24.441
3.165	100	-1	1	1	28.175
2.841	68	1	1	1	31.468
2.623	21	2	0	0	34.160
2.606	11	0	2	0	34.383
2.540	13	0	0	2	35.309
2.499	2	-2	0	1	35.900
2.3340	4	1	2	0	38.541
2.2845	1L	0	1	2	39.411
2.2527	1L	-2	1	1	39.990
2.2138	12	-1	1	2	40.725
2.1919	5	2	0	1	41.150
2.1805	5	-1	2	1	41.374

d(A)	I^{rel}	h	k	ℓ	2θ (°)
2.0203	7	2	1	1	44.826
1.9910	6	-2	0	2+	45.522
1.8593	2	-2	1	2	48.949
1.8481	18	2	2	0	49.266
1.8137	22	0	2	2	50.116
1.8038	13	-2	2	1	50.559
1.7830	5	-1	2	2	51.193
1.6937	11	0	0	3+	54.104
1.6772	1L	2	2	1	54.680
1.6571	11	3	1	0	55.400
1.6524	9	-3	1	1	55.570
1.6439	6	0	3	1	55.883
1.6100	7	-1	1	3+	57.163
1.5924	4	-1	3	1	57.861
1.5822	3	-2	2	2	58.268
1.5459	8	1	3	1	59.775
1.5393	7	-2	0	3	60.055
1.5095	5	3	1	1	61.367
1.4960	5	-3	1	2	61.984
1.4777	8	1	1	3	62.838
1.4520	1	3	2	0	64.079
1.4486	2	2	3	0	64.250
1.4343	1L	0	3	2	64.966
1.4262	2	-2	3	1	65.384
1.4201	6	0	2	3+	65.700
1.4165	4	-1	3	2	65.884
1.3615	1	2	3	1	68.912
1.3494	1L	3	2	1	69.620
1.3398	1L	-3	2	2	70.190
1.3253	2	-2	2	3	71.071
1.3217	4	-4	0	1	71.300
1.3113	1	4	0	0	71.950
1.3089	1	-2	3	2	72.104
1.3035	1L	0	4	0	72.450
1.3005	1L	3	1	2	72.642
1.2862	1L	-3	1	3	73.580
1.2700	2	0	0	4	74.682
1.2647	4	1	4	0	75.046
1.2455	1	-1	1	4	76.410
1.2321	1L	3	3	0	77.392
1.2230	1L	4	0	1	78.079
1.2127	1	0	3	3+	78.866

Received April 15, 1986 Accepted May 10, 1986