

ภาคผนวก ก

ไฟล์มาตรฐาน JCPDS หมายเลข 00-009-0169 (Beta-Tricalciumphosphate)

Name and formula

Reference code:	00-009-0169
Mineral name:	Whitlockite-Syn
PDF index name:	Calcium Phosphate
Empirical formula:	$\text{Ca}_3\text{O}_8\text{P}_2$
Chemical formula:	$\text{Ca}_3(\text{PO}_4)_2$

Crystallographic parameters

Crystal system:	Rhombohedral
Space group:	R-3c
Space group number:	167

a (?): 10.4290

b (?): 10.4290

c (?): 37.3800

Alpha (?): 90.0000

Beta (?): 90.0000

Gamma (?): 120.0000

Calculated density (g/cm³): 3.07

Measured density (g/cm³): 3.12

Volume of cell (10⁶ pm³): 3520.91

Z: 21.00

RIR: -

subfiles and quality

Subfiles:

- Inorganic
- Mineral
- Pharmaceutical
- Corrosion
- Common Phase
- Educational pattern
- Forensic

Quality: Indexed (I)

Comments

Color: Colorless, white, gray, yellow

Sample source: Sample obtained by heating a commercial sample

Structure: Nearly isostructural with cerite.

Optical data: A=1.626, B=1.629, Sign=-

Additional pattern: Validated by calculated pattern 42-577.

See ICSD 6191 (PDF 70-2065).

References

Primary reference: de Wolff, P., TechnischPhysischeDienst, Delft, The Netherlands., *ICDD Grant-in-Aid*, (1957)

Structure: Calvo, C., Gopal, R., *Am. Mineral.*, **60**, 120, (1975)

Optical data: *Dana's System of Mineralogy, 7th Ed.*, **II**, 684, (1951)

Peak list

No.	h	k	l	d [Å]	2Theta[deg]	I [%]
1	0	1	2	8.15000	10.847	12.0
2	1	0	4	6.49000	13.633	16.0
3	0	0	6	6.22000	14.228	6.0
4	1	1	0	5.21000	17.005	20.0
5	1	1	3	4.80000	18.469	2.0
6	2	0	2	4.39000	20.212	8.0
7	0	1	8	4.15000	21.394	4.0
8	0	2	4	4.06000	21.874	16.0
9	1	1	6	4.00000	22.206	4.0
10	1	0	10	3.45000	25.803	25.0
11	2	1	1	3.40000	26.189	4.0
12	1	2	2	3.36000	26.507	10.0

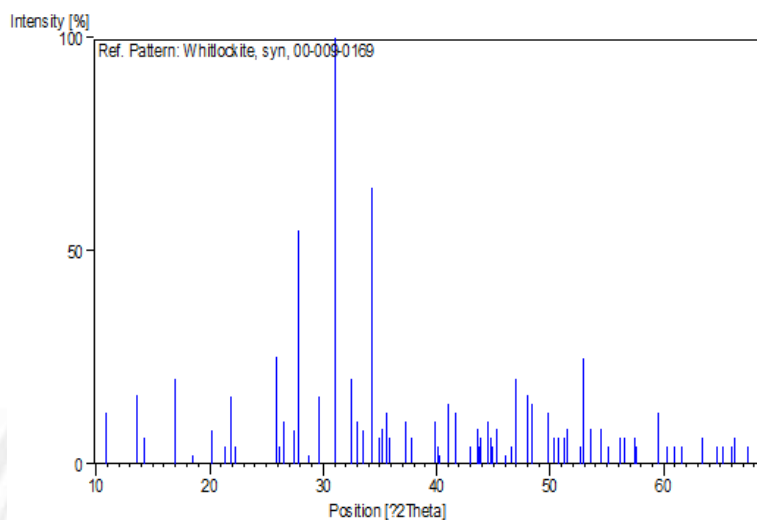
13	1	1	9	3.25000	27.421	8.0
14	2	1	4	3.21000	27.769	55.0
15	1	2	5	3.11000	28.681	2.0
16	3	0	0	3.01000	29.655	16.0
17	0	2	10	2.88000	31.027	100.0
18	1	2	8	2.75700	32.449	20.0
19	3	0	6	2.71000	33.027	10.0
20	1	1	12	2.67400	33.485	8.0
21	2	2	0	2.60700	34.372	65.0
22	0	1	14	2.56200	34.995	6.0
23	2	2	3	2.55300	35.122	8.0
24	2	1	10	2.52000	35.598	12.0
25	1	3	1	2.49900	35.907	6.0
26	1	2	11	2.40700	37.329	10.0
27	3	1	5	2.37500	37.851	6.0
28	1	0	16	2.26300	39.801	10.0
29	1	1	15	2.24900	40.059	4.0
30	0	4	2	2.24100	40.209	2.0
31	4	0	4	2.19500	41.089	14.0
32	3	0	12	2.16500	41.685	12.0

33	1	2	14	2.10300	42.974	4.0
34	0	0	18	2.07600	43.561	8.0
35	3	2	1	2.06800	43.738	4.0
36	2	3	2	2.06100	43.894	6.0
37	0	4	8	2.03300	44.531	10.0
38	3	2	4	2.02300	44.763	6.0
39	3	1	11	2.01700	44.903	4.0
40	2	2	12	2.00000	45.306	8.0
41	4	1	0	1.97000	46.035	2.0
42	4	1	3	1.94600	46.636	4.0
43	4	0	10	1.93300	46.969	20.0
44	2	3	8	1.89500	47.969	16.0
45	4	1	6	1.87900	48.404	14.0
46	0	1	20	1.83000	49.787	12.0
47	3	2	10	1.81200	50.315	6.0
48	5	0	2	1.79800	50.735	6.0
49	4	1	9	1.78100	51.254	6.0
50	0	5	4	1.77400	51.471	8.0
51	3	3	0	1.73800	52.618	4.0
52	2	0	20	1.72800	52.946	25.0

53	3	0	18	1.71100	53.514	8.0
54	5	0	8	1.68500	54.407	8.0
55	4	1	12	1.66500	55.116	4.0
56	2	3	14	1.63700	56.141	6.0
57	2	2	18	1.62500	56.593	6.0
58	4	2	8	1.60300	57.441	6.0
59	5	1	4	1.60000	57.559	4.0
60	5	1	7	1.55200	59.515	12.0
61	1	5	8	1.53200	60.372	4.0
62	2	1	22	1.52000	60.899	4.0
63	6	0	0	1.50500	61.571	4.0
64	1	5	11	1.46500	63.445	6.0
65	0	4	20	1.44000	64.678	4.0
66	0	5	16	1.42900	65.238	4.0
67	3	4	8	1.41400	66.017	4.0
68	5	2	6	1.40900	66.282	6.0
69	1	5	14	1.38700	67.473	4.0

Stick Pattern

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ไฟล์มาตรฐาน JCPDS หมายเลข 01-081-2200 (Barium ZirconiumTitanate)

Name and formula

Reference code: 01-081-2200
 ICSD name: Barium Titanium Oxide
 Empirical formula: BaO₃Ti
 Chemical formula: Ba (TiO₃)

Crystallographic parameters

Crystal system: Orthorhombic
 Space group: Amm2
 Space group number: 38
 a (?): 3.9874
 b (?): 5.6751
 c (?): 5.6901
 Alpha (?): 90.0000

Beta (?): 90.0000

Gamma (?): 90.0000

Calculated density (g/cm³): 6.01

Volume of cell (10⁶ pm³): 128.76

Z: 2.00

RIR: -

Status, subfiles and quality

Status: Diffraction data collected at high or low temperature

Subfiles: Inorganic

Corrosion

Modelled additional pattern

Quality: Calculated (C)

Comments

ICSD collection code: 073641

Test from ICSD: At least one TF implausible.

References

Primary reference: Calculated from ICSD using POWD-12++, (1997)

Structure: Kwei, G.H., Lawson, A.C., Billinge, S.J.L., Cheong, S.- W., *J. Phys. Chem.*, **97**, 2368, (1993) Peak list

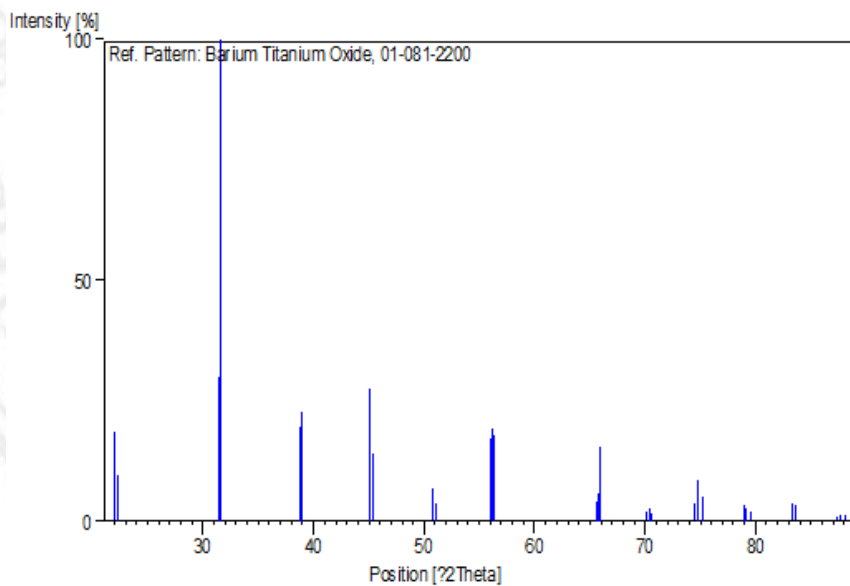
Peak list

No. h k l d [Å] 2Theta[deg] I [%]

1	0	1	1	4.01819	22.104	18.4
2	1	0	0	3.98740	22.277	9.5
3	0	0	2	2.84505	31.418	30.0
4	1	1	1	2.83034	31.585	100.0
5	1	0	2	2.31596	38.854	19.7
6	1	2	0	2.31191	38.925	22.7
7	0	2	2	2.00910	45.090	27.7
8	2	0	0	1.99370	45.457	13.8
9	0	1	3	1.79889	50.708	3.0
10	0	3	1	1.79421	50.850	6.7
11	2	1	1	1.78595	51.102	3.9
12	1	1	3	1.63975	56.038	17.3
13	1	3	1	1.63687	56.146	19.2
14	2	0	2	1.63272	56.301	17.8
15	0	0	4	1.42253	65.572	4.2
16	0	4	0	1.41877	65.767	5.7
17	2	2	2	1.41517	65.956	15.3
18	1	0	4	1.33982	70.189	2.0
19	1	4	0	1.33558	70.445	2.8
20	2	3	1	1.33403	70.539	1.8
21	0	2	4	1.27167	74.564	3.8
22	1	3	3	1.26968	74.701	8.5
23	3	1	1	1.26189	75.242	5.2
24	1	2	4	1.21155	78.958	3.6
25	1	4	2	1.20981	79.094	2.8

26	3	0	2	1.20420	79.536	2.1
27	2	0	4	1.15798	83.397	3.5
28	2	4	0	1.15596	83.575	3.4
29	0	1	5	1.11581	87.316	0.8
30	0	5	1	1.11309	87.583	0.8
31	2	3	3	1.11180	87.711	1.0
32	3	2	2	1.10851	88.038	1.0

Stick Pattern



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