APPENDIX

The Joint Committee for Powder Diffraction Standards (JCPDS) of CaO_2 (00-003-0865)

Name and formula

Reference code:	00-003-0865
PDF index name:	Calcium Oxide
Empirical formula:	CaO_2
Chemical formula:	CaO_2

Crystallographic parameters

Crystal system:	Tetragonal
Space group:	I4/mmm
Space group number:	139
a (?):	3.5400
b (?):	3.5400
c (?):	5.9100
Alpha (?):	90.0000
Beta (?):	90.0000
Gamma (?):	90.0000
Volume of cell (10^6 pm^3):	74.06
Z:	2.00
RIR:	-

Subfiles and Quality

Subfiles:	Inorganic
	Alloy, metal or intermetalic
	Superconducting Material
Quality:	Blank (B)

Comments

Color: White

General comments: Decomposition temperature 275๏.

Color from *Handbook of Chemistry and Physics*.

References

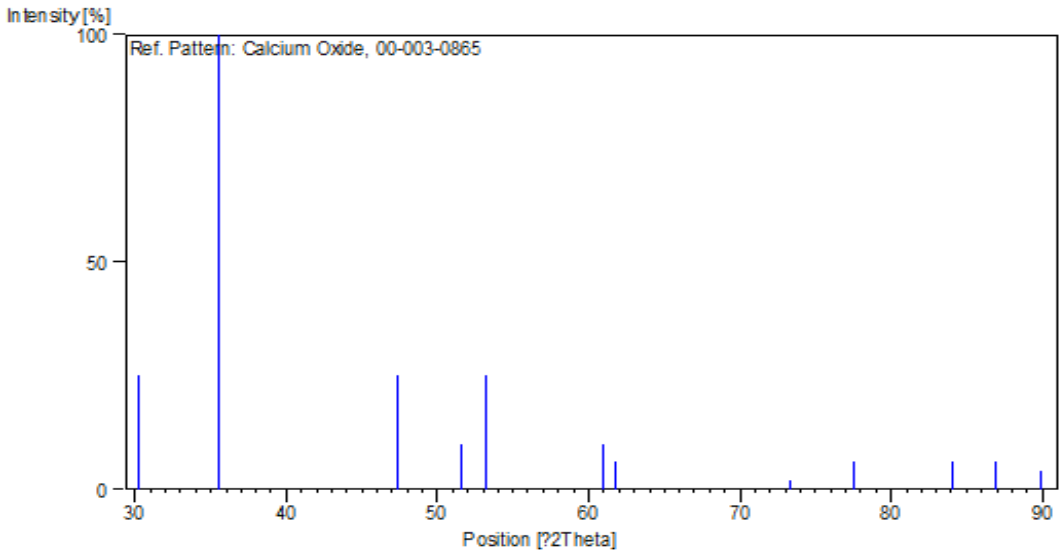
Primary reference: The Dow Chemical Company, Midland, Michigan, USA., *Private Communication*

Unit cell: Kotov, V., Raikhshtein, S., *Russ. J. Phys. Chem.*, **15**, 1057, (1941)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	0	0	2	2.95000	30.273	25.0
2	1	1	0	2.52000	35.598	100.0
3	1	1	2	1.92000	47.306	25.0
4	2	0	0	1.77000	51.596	10.0
5	1	0	3	1.72000	53.212	25.0
6	2	0	2	1.52000	60.899	10.0
7				1.50000	61.799	6.0
8	1	1	4	1.29000	73.330	2.0
9	2	1	3	1.23000	77.549	6.0
10	2	2	2	1.15000	84.107	6.0
11	3	1	0	1.12000	86.907	6.0
12				1.09000	89.934	4.0

Stick Pattern



The Joint Committee for Powder Diffraction Standards (JCPDS) of $CaCO_3$ (00-001-0837)

Name and formula

Reference code:	00-001-0837
Mineral name:	Calcite
PDF index name:	Calcium Carbonate Oxide
Empirical formula:	$CCaO_3$
Chemical formula:	$CaCO_3$

Crystallographic parameters

Crystal system:	Rhombohedral
Space group:	R-3c
Space group number:	167
a (?):	4.9830
b (?):	4.9830
c (?):	17.0190
Alpha (?):	90.0000
Beta (?):	90.0000

Gamma (?):	120.0000
Measured density (g/cm^3):	2.71
Volume of cell (10^6 pm^3):	365.97
Z:	2.00
RIR:	-

Status, subfiles and quality

Status:	Marked as deleted by ICDD
Subfiles:	Inorganic
	Mineral
	Pharmaceutical
Quality:	Blank (B)

Comments

Deleted by:	Deleted by NBS.
Color:	Various, white
General comments:	Melting point at 1025 atmospheres.
Optical data:	A=1.4864, B=1.658, Sign=-
Melting point:	1339
Unit cell:	Rhombohedral cell: a=6.361, a=46.7.

References

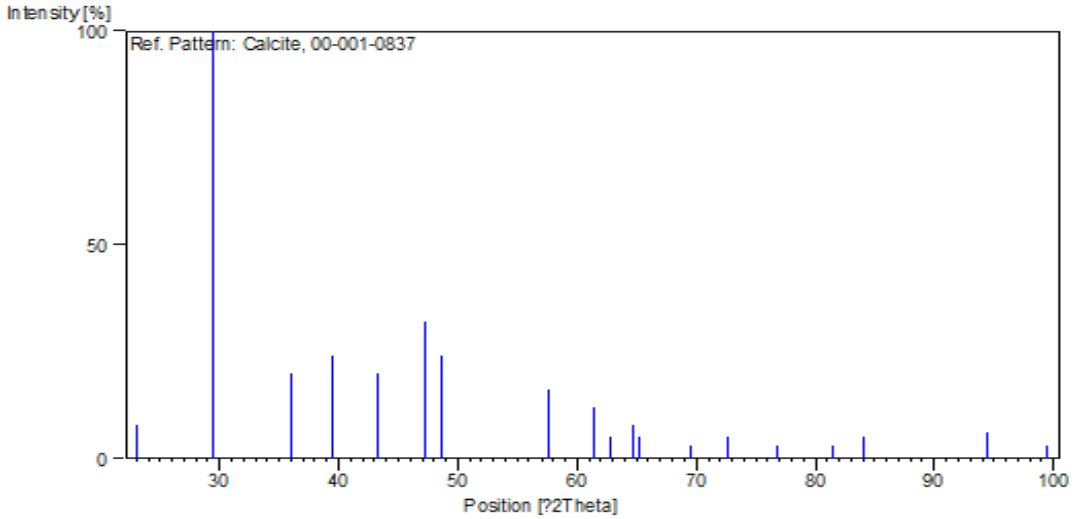
Primary reference:	Hanawalt. et al., *Anal. Chem.*, **10**, 475, (1938)
Unit cell:	*Archs. Sci. Geneve*

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	0	1	2	3.86000	23.022	8.0
2	1	0	4	3.04000	29.356	100.0
3	1	1	0	2.49000	36.041	20.0
4	1	1	3	2.28000	39.492	24.0
5	2	0	2	2.09000	43.254	20.0
6	0	2	4	1.92000	47.306	32.0
7	1	1	6	1.87000	48.652	24.0
8	1	2	2	1.60000	57.559	16.0

9	1	1	9	1.51000	61.345	12.0
10	1	2	5	1.48000	62.728	5.0
11	3	0	0	1.44000	64.678	8.0
12				1.43000	65.186	5.0
13	2	1	7	1.35000	69.583	3.0
14	1	2	8	1.30000	72.675	5.0
15	2	2	0	1.24000	76.809	3.0
16	2	1	10	1.18000	81.506	3.0
17	1	3	4	1.15000	84.107	5.0
18	4	0	4	1.05000	94.381	6.0
19	3	0	12	1.01000	99.401	3.0

Stick Pattern



The Joint Committee for Powder Diffraction Standards (JCPDS) of $CaCO_3$ (00-001-1032)

Name and formula

Reference code: 00-001-1032

PDF index name: Calcium Carbonate

Empirical formula: $CCaO_3$

Chemical formula: $CaCO_3$

Crystallographic parameters

Crystal system: Unknown

RIR: -

Status, subfiles and quality

Status: Marked as deleted by ICDD

Subfiles: Inorganic

Pharmaceutical

Quality: Blank (B)

Comments

Deleted by: see comments of Post October 1955.

References

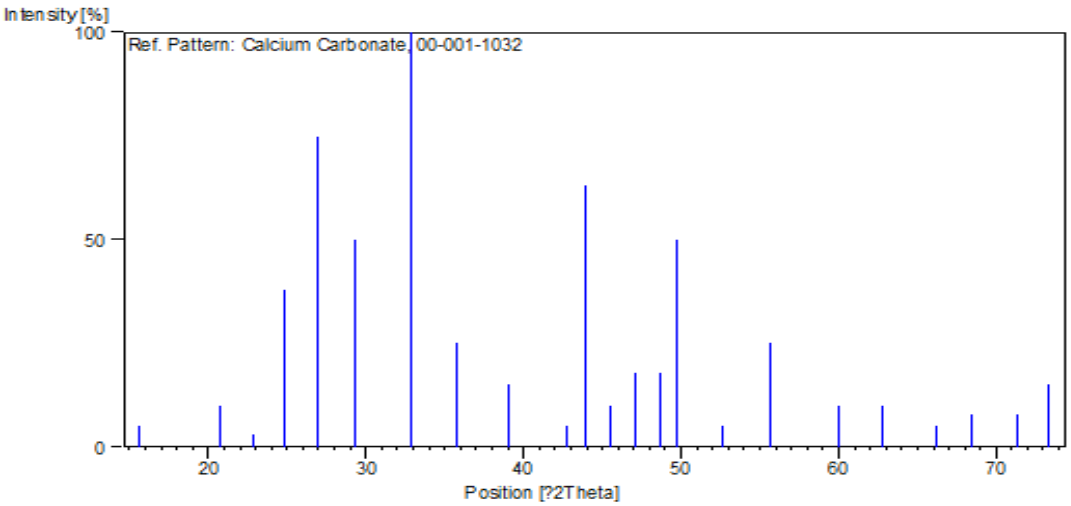
Primary reference: Hanawalt. et al., *Anal. Chem.*, **10**, 475, (1938)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1				5.70000	15.533	5.0
2				4.29000	20.688	10.0
3				3.90000	22.783	3.0
4				3.59000	24.780	38.0
5				3.30000	26.998	75.0
6				3.04000	29.356	50.0
7				2.73000	32.778	100.0
8				2.51000	35.744	25.0
9				2.30000	39.135	15.0
10				2.11000	42.824	5.0
11				2.06000	43.917	63.0
12				1.99000	45.547	10.0
13				1.93000	47.046	18.0
14				1.87000	48.652	18.0
15				1.83000	49.787	50.0
16				1.74000	52.553	5.0

17	1.65000	55.660	25.0
18	1.54000	60.026	10.0
19	1.48000	62.728	10.0
20	1.41000	66.229	5.0
21	1.37000	68.425	8.0
22	1.32000	71.403	8.0
23	1.29000	73.330	15.0

Stick Pattern



The Joint Committee for Powder Diffraction Standards (JCPDS) of $Ca(OH)_2$ (00-044-1481)

Name and formula

Reference code: 00-044-1481

Mineral name: Portlandite, syn

PDF index name: Calcium Hydroxide

Empirical formula: CaH_2O_2

Chemical formula: $Ca(OH)_2$

Crystallographic parameters

Crystal system: Hexagonal

Space group: P-3m1

Space group number:	164
a (?):	3.5899
b (?):	3.5899
c (?):	4.9160
Alpha (?):	90.0000
Beta (?):	90.0000
Gamma (?):	120.0000
Calculated density (g/cm^3):	2.24
Volume of cell (10^6 pm^3):	54.87
Z:	1.00
RIR:	2.90

Subfiles and Quality

Subfiles:	Inorganic Mineral Cement and Hydration Product Common Phase Forensic Pharmaceutical
Quality:	Star (S)

Comments

Deleted by:	Deleted by 4-733 which is satisfactory.
Color:	White
General comments:	Average relative standard deviation in intensity of the ten strongest reflections for three specimen mounts = 2.2%.
Sample source:	Sample obtained from Sigma Chemical Co.
Optical data:	A=1.545, B=1.574, Sign=-
Additional pattern:	Validated by a calculated pattern.

References

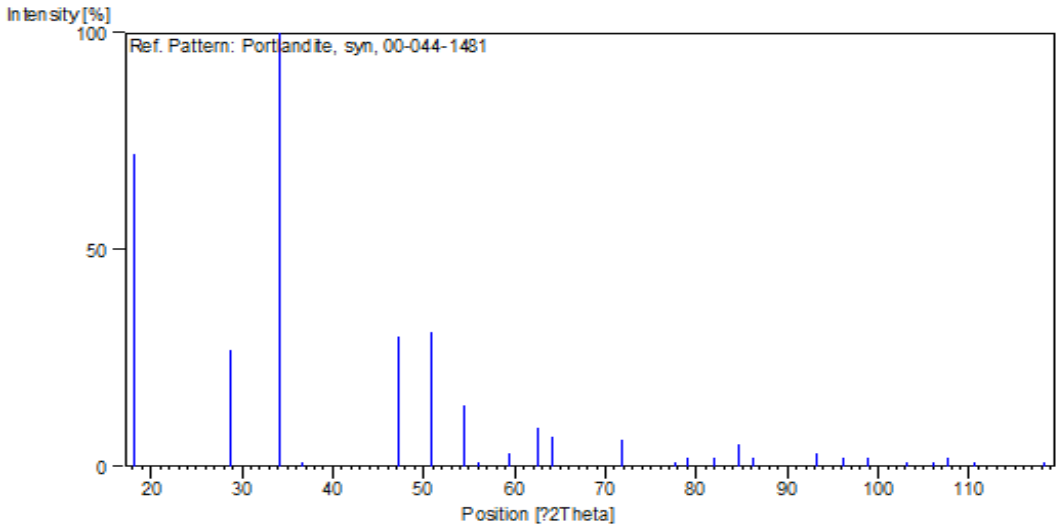
Primary reference:	Martin, K., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA., *ICDD Grant-in-Aid*, (1992)

Optical data: Winchell, A., Winchell, H., *Microscopic Character of Artificial Inorg. Solid Sub.*, 69, (1964)

Peak list

No.	h	k	l	d [A]	2Theta[deg]	I [%]
1	0	0	1	4.92200	18.008	72.0
2	1	0	0	3.11100	28.672	27.0
3	1	0	1	2.62700	34.102	100.0
4	0	0	2	2.45800	36.527	1.0
5	1	0	2	1.92710	47.121	30.0
6	1	1	0	1.79540	50.813	31.0
7	1	1	1	1.68640	54.358	14.0
8	0	0	3	1.63830	56.092	1.0
9	2	0	0	1.55410	59.426	3.0
10	2	0	1	1.48200	62.634	9.0
11	1	0	3	1.44890	64.233	7.0
12	2	0	2	1.31350	71.811	6.0
13	0	0	4	1.22860	77.654	1.0
14	1	1	3	1.20980	79.095	2.0
15	2	1	0	1.17520	81.910	2.0
16	1	0	4	1.14290	84.751	5.0
17	2	0	3	1.12740	86.197	2.0
18	2	1	2	1.06010	93.209	3.0
19	3	0	0	1.03630	96.030	2.0
20	1	1	4	1.01390	98.882	2.0
21	0	0	5	0.98330	103.143	1.0
22	2	0	4	0.96410	106.066	1.0
23	2	1	3	0.95470	107.579	2.0
24	1	0	5	0.93739	110.521	1.0
25	2	2	0	0.89740	118.268	1.0

Stick Pattern



Studied surface area of CaO_2 powders were synthesized in mild condition by The Brunauer–Emmett–Teller (BET)

Instrument: Model Autosorb 1 MP, Quantachrome

Condition: Surface area determination

P/Po: 5 points (BET)

Adsorbate: Nitrogen gas

Out gas temperature: 250 ^{o}C

Out gas time: 5 hours

Operating time: 42.2-43.9 min Total: 5.71-5.73 hours/sample

Table 6. Multipoint BET

P/Po	Volume [cc/g] STP	1/(W((Po/P)-1))
1.0846e-01	2.6801	3.632E+01
1.6120e-01	3.1090	4.946E+01
2.1135e-01	3.3898	6.326E+01
2.6121e-01	3.7547	7.534E+01
3.1105e-01	4.1019	8.807E+01

Area = 1.316E+01 M^2/g

Slop = 2.561E+02

Y – Intercept = 8.539E+00

Correlation Coefficient = 0.999849

C = 3.099E+01

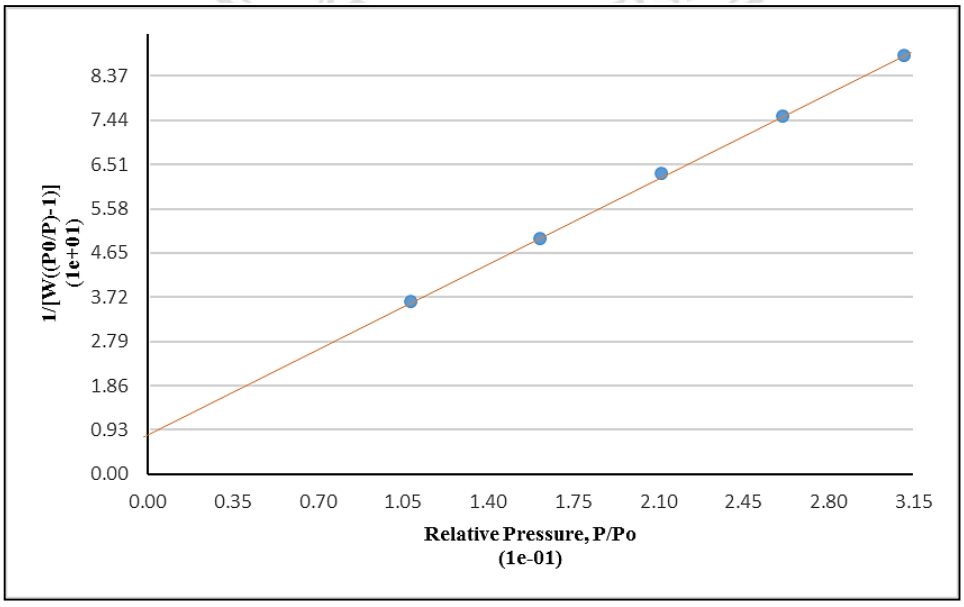


Figure 29. BET Plot

CURRICULUM VITAE

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Publication Pongpen Kaewdee, Nopakarn Chandet and Gobwute Rujijanagul, "Multicatalytic properties of nanoparticle CaO_2 synthesized by a novel, simple and economical method for wastewater treatment", Catalysis Communication, Vol.84, 5 September 2016, Pages 151-154.

Pongpen Kaewdee, Chamnan Randorn, "Dye Waste treatment by high purity nanoparticle CaO2 powders prepared by a novel and economical method", The Fifth International Conference on Human-Environment System (ICHES 2016), 29 October – 3 November 2016, Japan. (Oral presentation, Proceeding).