APPENDIX A

SELECTED DATA SETS FROM THE POWDER DIFFRACTION FILE

Selected data sets from the 1995 Powder Diffraction File-2 (Set 45), release A6, published by the International Centre for Diffraction Data, are given in Tables A.1 to A.15.

Table A.1: Data set no. 5-378 from the Powder Diffraction File (Set 45)

Pattern : 5-378	***Radiation :*** 1.540560		***Quality :*** Indexed			
$BaCO_3$ Witherite, syn / Barium Carbonate		***d (Å)***	***I***	***h***	***k***	***l***
Lattice: Orthorhombic		4.5600	9	1	1	0
S.G.: Pmcn (62)		4.4500	4	0	2	0
Mol. weight = 197.34		3.7200	100	1	1	1
Volume [CD] = 304.24		3.6600	53	0	2	1
Dx = 4.308		3.2150	15	0	0	2
I/Icor = 4.20		3.0250	4	0	1	2
		2.7490	3	1	0	2
a = 5.31400 ***b*** = 8.90400 ***c*** = 6.43000		2.6560	11	2	0	0
a/b = 0.59681 ***c/b*** = 0.72215		2.6280	24	1	1	2
Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00		2.5900	23	1	3	0
Z= 4		2.2810	6	2	2	0
		2.2260	2	0	4	0
OPTICAL DATA: A=1.530, B=1.679, Q=1.680, Sign=-, 2V=9 deg.(calc.) COLOR: Colorless SAMPLE SOURCE OR LOCALITY: Sample from Mallinckrodt Chemical Works. ANALYSIS: Spectroscopic analysis: showed <0.01 % Al, Ca, Na, Sr; <0.001% Cu, Fe, Mg, Pb. TEMP. OF DATA COLLECTION: Pattern taken at 26 °C. ADDITIONAL PATTERN: To replace 1-506.		2.1500	28	2	2	1
		2.1040	12	0	4	1
		2.0480	10	2	0	2
		2.0190	21	1	3	2
		1.9400	15	1	1	3
		1.8590	3	2	2	2
		1.8300	2	0	4	2
		1.7370	2	3	1	0
		1.7060	1	2	4	0
		1.6770	5	3	1	1
		1.6490	4	2	4	1
		1.6330	4	1	5	1
		1.5630	3	2	2	3
		1.5430	1	0	4	3
		1.5210	4	3	3	0
		1.5080	2	2	4	2
		1.4840	1	0	6	0
		1.3750	6	3	3	2
		1.3660	4	1	3	4
		1.3480	4	0	6	2
		1.3350	3	2	4	3
		1.3280	4	4	0	0
		1.2950	3	2	6	0
		1.2480	1	2	3	4
		1.2330	2	3	5	1
		1.2150	1	1	7	1
		1.2020	1	1	2	5
		1.2020	1	2	6	2
		1.1703	1	2	4	4
		1.1335	2	4	3	2
		1.0951	2	0	8	1
		1.0951	2	4	2	3
CAS: 14941 -39-0 *Natl. Burl Stand. (U.S.), Circ.539, volume 2, page 54, (1953) primary reference: Swanson, Fuyat.						
Radiation: CuKα1	**Filter:** Beta					
Lambda: 1.54050	**d-sp:** Not given					
SS/FOM: F30= 35(0.0123,7)	**No standard**					

Table A.2: Data set no. 17-306 from the Powder Diffraction File (Set 45)

Pattern : 17-306 ***Radiation :*** 1.540560 ***Quality :*** High

$BaAl_2O_4$

Barium Aluminium Oxide

Lattice: Hexagonal

S.G.: P6322 (182)

Mol. weight = 255.29

Volume [CD]= 831.19

Dx= 4.080

I/Icor = 4.40

a = 10.44700 ***b*** = 10.44700 ***c*** = 8.79400

a/b = 1.00000 ***c/b*** = 0.84177

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 120.00

Z= 8

OPTICAL DATA: B=1.675
COLOR: Colorless
ANALYSIS: Spectrographic analysis showed the following major impurities: 0.01 -0.1 % each of Ca, Si, and V.
TEMP. OF DATA COLLECTION: Pattern at 25 °C.
SAMPLE PREPARATION: Prepared from gamma- Al_2O_3 and $BaCO_3$. Heated at 1200 °C for 1 1/2 hours.
ADDITIONAL DIFFRACTION LINE(S): Plus 4 reflections to 0.7882.

*Natl. Burl Stand. (U.S.) Monogr. 25, volume 5, page 11, (1967) primary reference:

Radiation: CuKα1 **Filter:** Beta

Lambda: 1.54050 **d-sp:** Not given

SS/FOM: F30=35(0.0084,10) **Internal standard:** Ag

d (Å)	*I*	*h*	*k*	*l*	*d* (Å)	*I*	*h*	*k*	*l*
4.5250	45	2	0	0	0.9532	1	6	2	6
4.4010	6	0	0	2	0.9431	1	9	1	1
4.0220	10	2	0	1	0.9386	1	6	4	4
3.1530	100	2	0	2	0.9247	2	4	2	8
2.6110	40	2	2	0	0.9005	1	8	2	4
2.5050	3	2	2	1	0.8953	1	8	0	6
2.4610	2	2	0	3	0.8883	1	6	0	8
2.4130	1	3	1	1	0.8861	1	10	0	2
2.2620	11	4	0	0	0.8706	1	6	6	0
2.2460	25	2	2	2	0.8632	1	2	0	10
2.1990	10	0	0	4	0.8547	1	10	1	1
2.1360	1	1	0	4	0.8470	1	6	4	6
2.0111	19	4	0	2	0.8410	1	4	4	8
1.9774	12	2	0	4	0.8391	2	8	4	2
1.9505	1	2	2	3	0.8367	1	10	0	4
1.7911	1	4	0	3	0.8334	1	2	2	10
1.7098	5	4	2	0	0.8268	2	6	2	8
1.6822	10	2	2	4	0.8188	2	8	2	6
1.6391	1	2	0	5	0.8125	1	10	2	0
1.5935	18	4	2	2	0.8090	1	10	2	1
1.5764	7	4	0	4	0.7990	2	10	2	2
1.5078	8	6	0	0	0.7970	2	8	4	4
1.4771	1	4	2	3	0.7882	1	8	0	8
1.4660	1	0	0	6					
1.4263	1	6	0	2					
1.3944	3	2	0	6					
1.3890	1	4	0	5					
1.3628	1	6	1	1					
1.3496	6	4	21	4					
1.3057	3	4	4	0					
1.2782	5	2	2	6					
1.2547	1	6	2	0					
1.2516	2	4	4	2					
1.2435	4	6	0	4					
1.2299	1	4	0	6					
1.2262	1	4	2	5					
1.2063	6	6	2	2					
1.1536	1	6	2	3					
1.1308	1	8	0	0					
1.1228	2	4	4	4					
1.1129	2	4	2	6					
1.0952	2	8	0	2					
1.0898	2	6	2	4					
1.0683	2	2	0	8					
1.0549	1	8	0	3					
1.0511	1	6	0	6					
1.0379	1	6	4	0					
1.0216	1	6	2	5					
1.0132	1	2	2	8					
1.0100	2	6	4	2					
1.0056	1	8	0	4					
0.9885	1	4	0	8					
0.9872	2	8	2	0					
0.9783	1	6	4	3					
0.9750	1	4	4	6					
0.9632	1	8	2	2					

Table A.3: Data set no. 21-806 from the Powder Diffraction File (Set 45)

Pattern : 21-806 ***Radiation :*** 1.540560 ***Quality :*** Indexed

$BaAl_2SiO_6$

Barium Aluminium Silicate

Lattice: Hexagonal

S.G.: P63/m (176)

Mol. weight = 315.38

Volume [CD] = 1595.48

Dx = 0.328

a = 9.95500 ***b*** = 9.95500 ***c*** = 18.59000

a/b = 1.00000 ***c/b*** = 1.86740

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 120.00

OPTICAL DATA: A=1.628, Q=1.636, Sign=+, 2V=0-30 deg.
MELTING POINT: 1400 °C
SAMPLE PREPARATION: Synthetic, solid state reaction at 1380 °C for 7 days.
GENERAL COMMENTS: Unit cell data refined from powder spacings.

*Neues Jahrb. Mineral., Monatsh., page 15, (1969)
primary reference: Kockel, Oehischlegel.

Radiation:

Filter: Not specified

d-sp: Guinier

SS/FOM: F30= 51 (0.0183,3)

No standard

d (Å)	*I*	*h*	*k*	*l*	*d (Å)*	*I*	*h*	*k*	*l*
9.3100	12	0	0	2	1.9110	16	1	1	9
8.6500	8	1	0	0	1.8950	25	3	1	6
7.8500	45	1	0	1	1.8850	14	3	2	3
6.3500	8	1	0	2	1.8820	14	4	1	0
5.0300	30	1	0	3	1.8730	12	4	1	1
4.9800	35	1	1	0	1.8650	10	4	0	5
4.8100	60	1	1	1	1.8450	12	4	1	2
4.6500	20	0	0	4	1.8220	16	3	2	4
4.3100	6	2	0	0	1.8080	10	3	0	8
4.1900	30	2	0	1	1.7790	8	3	1	7
4.0900	4	1	0	4	1.7470	18	3	2	5
3.9100	8	2	0	2	1.7380	4	1	1	10
3.8800	20	1	1	3	1.7180	8	5	0	1
3.5400	90	2	0	3	1.6960	6	5	0	2
3.4200	16	1	0	5	1.6810	8	4	1	5
3.4000	45	1	1	4	1.6760	12	3	0	9
3.2600	35	2	1	0	1.6690	20	3	2	6
3.2100	75	2	1	1	1.6620	4	5	0	3
3.1000	40	0	0	6	1.6590	2	3	3	0
3.0800	100	2	1	2	1.6530	4	3	3	1
2.9810	75	1	1	5	1.6340	4	3	3	2
2.9190	8	1	0	6	1.6310	6	4	2	0
2.8840	14	2	1	3	1.6240	4	4	2	1
2.8730	35	3	0	0	1.6190	4	5	0	4
2.8400	12	3	0	1	1.6100	4	4	1	6
2.8170	18	2	0	5	1.6040	20	4	2	2
2.7460	8	3	0	2	1.5660	10	5	0	5
2.6690	60	2	1	4	1.5490	4	0	0	12
2.6330	20	1	1	6	1.5380	8	4	2	4
2.6070	8	3	0	3	1.5290	4	5	1	2
2.5420	30	1	0	7	1.5040	12	5	1	3
2.5190	20	2	0	6					
2.4890	2	2	2	0					
2.4550	12	2	1	5					
2.4480	6	3	0	4					
2.4060	10	2	2	2					
2.3730	30	3	1	1					
2.3490	2	1	1	7					
2.3290	2	0	0	8					
2.3170	45	3	1	2					
2.2740	2	3	0	5					
2.2580	35	2	0	7					
2.2480	45	2	1	6					
2.2320	50	3	1	3					
2.1560	6	4	0	0					
2.1430	14	4	0	1					
2.1280	14	3	1	4					
2.1100	6	3	0	6					
2.0610	8	2	1	7					
2.0370	16	4	0	3					
2.0110	18	3	1	5					
1.9680	35	3	2	1					
1.9560	10	4	0	4					
1.9500	6	3	0	7					
1.9430	6	2	2	6					
1.9360	12	3	2	2					

Table A.4: Data set no. 25-1476 from the Powder Diffraction File (Set 45)

Pattern : 25-1476 ***Radiation :*** 1.540560 ***Quality :*** Indexed

$BaFe_4O_7$ / $BaO.2Fe_2O_3$

Barium Iron Oxide

Lattice: Hexagonal

S.G.: P63/m (176)

Mol. weight = 472.71

Volume [CD] = 318.46

Dx = 4.930

Dm = 4.930

a = 5.16000 ***b*** = 5.16000 ***c*** = 13.81100

a/b = 1.00000 ***c/b*** = 2.67655

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 120.00

Z= 2

SAMPLE PREPARATION: Sample was prepared by aqueous hydrothermal treatment of alpha- Fe_2O_3 in $Ba(OH)_2$ solution.
GENERAL COMMENTS: Preferred orientation was unavoidable.

*Acta Crystallogr., Sec. B, volume 29, page 832, (1973) primary reference Okamoto et al.

Radiation: CoKα **Filter:** Beta

Lambda: 1.79020 **d-sp:** Not given

SS/FOM: F22= 14(0.0400,4) **No standard**

d (Å)	*I*	*h*	*k*	*l*
6.9000	45	0	0	2
4.2600	60	1	0	1
3.4600	70	0	0	4
3.2100	60	1	0	3
2.7300	95	1	0	4
2.5800	35	1	1	0
2.3500	20	1	0	5
2.3030	100	0	0	6
2.2520	8	1	1	3
2.2070	8	2	0	1
2.0690	20	1	1	4
2.0120	8	2	0	3
1.8770	25	2	0	4
1.8060	40	1	0	7
1.7270	65	0	0	8
1.6770	6	2	1	1
1.5870	8	2	1	3
1.5180	12	2	1	4
1.4910	8	3	0	0
1.4800	8	3	0	1
1.4530	8	1	0	9
1.4350	40	1	1	8

Table A.5: Data set no. 25-1477 from the Powder Diffraction File (Set 45)

Pattern : 25-1477 ***Radiation :*** 1.540560 ***Quality :*** Indexed

$Ba_3Fe_2O_6$ / $3BaO.Fe_2O_3$

Barium Iron Oxide

Lattice: Cubic

S.G.: (0)

Mol. weight = 619.68

Volume [CD]= 4694.37

Dx = 5.261

Dm = 5.200

a = 16.74400 ***b*** = 16.74400 ***c*** = 16.74400

a/b = 1.00000 ***c/b*** = 1.00000

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

Z= 24

SAMPLE PREPARATION: Formed at pressure 200 kg/cm^{-2} and 1000-1200 °C.
GENERAL COMMENTS: Unstable at <800 °C.

*Ann. Chim. (Rome), volume 62, page 641, (1972) primary reference: Montorsi, Brisi.

Radiation: Co **Filter:** Not specified

Lambda: 1.78897 **d-sp:** Not given

SS/FOM: F30= 14(0.0310,6) **No standard**

d (Å)	*I*	*h*	*k*	*l*
5.0400	2	3	1	1
4.4700	2	3	2	1
4.1800	20	4	0	0
3.8300	10	3	3	1
3.6500	3	4	2	1
3.4200	1	4	2	2
3.2200	15	5	1	1
3.1000	5	5	2	0
3.0500	2	5	2	1
2.9580	100	4	4	0
2.9100	2	4	4	1
2.8320	3	5	3	1
2.7500	1	6	1	0
2.6140	1	5	4	0
2.5520	1	5	3	3
2.4960	1	6	3	0
2.4160	18	4	4	4
2.3420	6	5	5	1
2.2780	1	7	2	1
2.2360	6	6	4	2
2.1800	7	7	3	1
2.1260	1	6	5	1
2.0920	35	8	0	0
2.0760	1	7	4	0
2.0440	5	7	3	3
2.0020	1	6	5	3
1.9740	3	6	6	0
1.9340	2	7	5	1
1.9080	3	8	3	2
1.8730	5	8	4	0
1.8380	2	9	1	1
1.7550	4	9	3	1
1.7080	30	8	4	4
1.6830	1	7	7	1
1.6660	3	10	1	0
1.6190	6	9	5	1
1.5960	1	10	3	1
1.5480	2	9	6	0
1.4800	8	8	8	0
1.4640	4	9	7	1
1.4360	2	10	6	0

Table A.6: Data set no. 25-75 from the Powder Diffraction File (Set 45)

Pattern : 25-75 ***Radiation :*** 1.540560 ***Quality :*** High

$Ba_3Al_2O_6$

Barium Aluminium Oxide

Lattice: Cubic

S.G.: Pa3 (205)

Mol. weight = 561.95

Volume [CD]= 4471.74

Dx = 5.008

I/Icor = 1.20

a = 16.47500 ***b*** = 16.47500 ***c*** = 16.47500

a/b = 1.00000 ***c/b*** = 1.00000

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

Z= 24

COLOR: Colorless
GENERAL COMMENTS: Pattern at 25 °C.
SAMPLE PREPARATION: The sample was prepared by A.E. Moore of the Cement and Concrete Association by heating $BaCO_3$ and Al_2O_3 in a Pt crucible at 1400 °C.
ADDITIONAL PATTERN: To replace 14-106 and 15-331.

*Natl. Burl Stand. (U.S.) Monogr.25. volume 12, page 7, (1975) primary reference:
*Natl. Burl Stand. (U.S.) Monogr. 25, unit cell data: Ibid.
*Natl. Burl Stand. (U.S.) Monogr. 25, optical data: Ibid.

Radiation: CuKα1 **Filter:** Monochromator crystal

Lambda: 1.54060 **d-sp:** Not given

SS/FOM: F30= 49(0.0115,5) **Internal standard:** W

d (Å)	*I*	*h*	*k*	*l*	*d* (Å)	*I*	*h*	*k*	*l*
5.8200	3	2	2	0	1.4561	9	8	8	0
4.9650	3	3	1	1	1.4392	4	9	7	1
4.4070	1	3	2	1	1.4239	2	9	7	2
4.1200	35	4	0	0	1.4128	3	10	6	0
3.9940	1	4	1	0	1.4075	3	4	11	0
3.7780	9	3	3	1	1.3977	2	9	7	3
3.5940	2	4	2	1	1.3878	2	11	4	2
3.5130	2	3	3	2	1.3825	3	9	6	5
3.3620	3	4	2	2	1.3731	4	12	0	0
3.1690	13	5	1	1	1.3591	4	11	5	1
3.0570	6	2	5	0	1.3497	3	10	7	0
3.0070	14	5	2	1	1.3362	4	12	2	2
2.9110	100	4	4	0	1.3233	2	11	5	3
2.8700	3	4	4	1	1.3105	3	11	6	1
2.7840	2	5	3	1	1.3025	6	12	4	0
2.6730	2	6	1	1	1.2906	4	9	9	1
2.5740	1	4	5	0	1.2825	3	10	8	1
2.5430	2	5	4	1	1.2598	6	11	7	1
2.5120	2	5	3	3	1.2524	4	2	13	0
2.4570	2	6	3	0	1.2491	4	11	7	2
2.3770	20	4	4	4	1.2418	5	12	4	4
2.3060	7	5	5	1	1.2315	4	11	7	3
2.2860	1	6	4	0	1.2246	4	10	9	0
2.2630	4	2	7	0					
2.2010	5	6	4	2					
2.1450	5	7	3	1					
2.1100	1	6	5	0					
2.0590	30	8	0	0					
2.0280	1	7	4	1					
2.0120	6	7	3	3					
1.9820	1	8	2	1					
1.9690	2	6	5	3					
1.9410	5	6	6	0					
1.9160	2	8	3	1					
1.9020	3	7	5	1					
1.8780	3	8	3	2					
1.8420	15	8	4	0					
1.8080	5	9	1	1					
1.7880	2	2	9	0					
1.7760	2	9	2	1					
1.7460	1	8	5	0					
1.7270	3	9	3	1					
1.7080	1	8	5	2					
1.6810	20	8	4	4					
1.6638	2	9	4	1					
1.6557	4	7	7	1					
1.6397	4	9	4	2					
1.6151	2	10	2	0					
1.5926	6	9	5	1					
1.5706	3	10	3	1					
1.5367	2	9	5	3					
1.5234	3	6	9	0					
1.5039	2	10	4	2					
1.4855	2	11	1	1					
1.4736	2	2	11	0					
1.4680	2	11	2	1					

Table A.7: Data set no. 26-1402 from the Powder Diffraction File (Set 45)

Pattern : 26-1402 ***Radiation :*** 1.540560 ***Quality :*** High

$BaSiO_3$ / $BaO.SiO_2$

Barium Silicate

Lattice: Orthorhombic

S.G.: Pmmm (47)

Mol. weight = 213.41

Volume [CD] = 320.34

Dx = 4.425

I/Icor = 2.60

a = 5.61820 ***b*** = 12.44500 ***c*** = 4.58160

a/b = 0.45144 ***c/b*** = 0.36815

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

Z= 4

COLOR: Colorless
SAMPLE PREPARATION: This form was prepared by repeated grindings and heating of a 1:1 molar mixture of $Ba(OH)_2$ and silica gel at about 1100 °C. A second form occurs below about 990 °C.
GENERAL COMMENTS: Pattern made at 25 °C.
ADDITIONAL PATTERN: To replace 6-247, 12-651 and 21-83.
STRUCTURE: Isostructural with $BaGeO_3$ and NH_4BeF_3.

*Natl. Burl Stand. (U.S.) Monogr. 25, volume 13, page 8, (1976) primary reference:

Radiation: Cu

Lambda: 1.54056

SS/FOM: F30= 38(0.0158,5)

Filter: Monochromator crystal

d-sp: Not given

No standard

d (Å)	*I*	*h*	*k*	*l*	*d (Å)*	*I*	*h*	*k*	*l*
6.2300	2	0	2	0	1.3958	4	4	1	0
5.1200	14	1	1	0	1.3901	5	3	6	0
4.1740	11	1	2	0	1.3690	3	3	3	2
3.6930	35	0	2	1	1.3629	6	1	7	2
3.5520	15	1	0	1	1.3490	1	2	6	2
3.4180	100	1	1	1	1.3433	1	4	0	1
3.3390	65	1	3	0	1.3347	4	4	1	1
3.1120	55	0	4	0	1.3304	5	4	3	0
2.8080	25	2	0	0	1.3145	4	3	4	2
2.7400	10	2	1	0	1.3126	4	4	2	1
2.7230	10	1	4	0	1.3046	4	2	8	1
2.6990	14	1	3	1	1.2886	4	1	9	1
2.5740	8	0	4	1	1.2775	5	4	3	1
2.3530	17	2	1	1	1.2688	3	1	5	3
2.3420	11	1	4	1	1.2548	2	1	8	2
2.3250	4	2	3	0	1.2444	2	0	10	0
2.2930	17	0	0	2	1.2409	2	3	7	1
2.2350	25	2	2	1	1.2304	2	0	6	3
2.1860	2	0	5	1	1.2231	2	4	5	0
2.1230	1	1	0	2	1.2009	1	0	10	1
2.0850	12	2	4	0					
2.0750	20	0	6	0					
2.0390	30	1	5	1					
2.0070	5	1	2	2					
1.9460	2	1	6	0					
1.8970	8	2	4	1					
1.8890	20	1	3	2					
1.8629	4	2	5	0					
1.8459	10	0	4	2					
1.7932	6	3	2	0					
1.7766	6	0	7	0					
1.7588	5	2	1	2					
1.7541	4	1	4	2					
1.7337	7	3	0	1					
1.7174	4	3	1	1					
1.7067	5	3	3	0					
1.6950	15	1	7	0					
1.6685	2	2	6	0					
1.6328	2	2	3	2					
1.6151	1	1	5	2					
1.6046	4	3	4	0					
1.6002	4	3	3	1					
1.5682	4	2	6	1					
1.5554	1	0	8	0					
1.5427	4	2	4	2					
1.5387	4	0	6	2					
1.5144	7	3	4	1					
1.4989	2	1	8	0					
1.4836	4	0	2	3					
1.4734	6	1	0	3					
1.4649	4	1	1	3					
1.4458	3	2	5	2					
1.4350	3	1	2	3					
1.4280	6	2	7	1					
1.4247	3	1	8	1					
1.4126	4	3	2	2					

Table A.8: Data set no. 26-1403 from the Powder Diffraction File (Set 45)

Pattern : 26-1403 ***Radiation :*** 1.540560 ***Quality :*** Indexed

Ba_2SiO_4 / $2BaO.SiO_2$

Barium Silicate

Lattice: Orthorhombic

S.G.: Pnam (62)

Mol. weight = 366.74

Volume[CD]= 445.48

Dx = 5.468

I/Icor = 1.80

a = 7.50800 ***b*** = 10.21400 ***c*** = 5.80910

a/b = 0.73507 ***c/b*** = 0.56874

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

Z= 4

GENERAL COMMENTS: Pattern at 25 °C.
SAMPLE PREPARATION: Prepared by heating a 2:1 molar mixture of $BaCO_3$ and H_2SiO_3 at 1000 °C for 18 hours, grinding and reheating at 1400 °C for 2 hours.
ADDITIONAL PATTERN: To replace 6-366.

*Natl. Burl Stand. (U.S.) Monogr. 25, volume 13, page 12, (1976) primary reference:
*Natl. Burl Stand. (U.S.) Monogr. 25, unit cell data:
Ibid.
*Natl. Burl Stand. (U.S.) Monogr. 25, optical data:
Ibid.

Radiation: Cu

Lambda: 1.54056

SS/FOM: F30= 61 (0.0105,4)

Filter: Monochromator crystal

d-sp: Not given

Internal standard: Ag

d (Å)	*I*	*h*	*k*	*l*	*d* (Å)	*I*	*h*	*k*	*l*
5.1100	10	0	2	0	1.3367	5	5	3	1
4.2200	16	1	2	0					
4.2000	25	1	1	1					
3.5240	14	2	1	0					
3.4150	80	1	2	1					
3.1530	25	2	0	1					
3.0980	20	1	3	0					
3.0220	70	2	2	0					
3.0170	100	2	1	1					
2.9380	95	0	3	1					
2.9050	70	0	0	2					
2.6830	13	2	2	1					
2.5540	9	0	4	0					
2.5250	20	0	2	2					
2.4310	40	3	1	0					
2.3930	20	1	2	2					
2.2970	5	2	0	2					
2.2420	20	3	1	1					
2.2330	19	1	4	1					
2.1200	20	1	3	2					
2.0950	30	2	2	2					
2.0170	12	3	3	0					
1.9840	6	2	4	1					
1.9710	16	1	5	0					
1.9280	4	0	5	1					
1.9180	2	0	4	2					
1.9040	17	2	3	2					
1.8770	3	4	0	0					
1.8640	25	3	1	2					
1.8440	4	1	1	3					
1.7950	3	2	5	0					
1.7880	6	3	4	0					
1.7860	5	4	0	1					
1.7594	25	4	1	1					
1.7203	5	2	0	3					
1.7084	35	3	4	1					
1.6970	14	2	1	3					
1.6832	14	0	3	3					
1.6566	16	3	3	2					
1.6438	6	4	3	0					
1.6309	16	2	2	3					
1.5967	5	1	6	1					
1.5767	2	4	0	2					
1.5507	4	2	6	0					
1.5115	6	1	4	3					
1.5066	6	4	2	2					
1.4976	6	2	6	1					
1.4684	4	0	6	2					
1.4639	2	4	4	1					
1.4524	9	0	0	4					
1.4396	8	5	1	1					
1.4301	7	4	3	2					
1.4151	6	0	7	1					
1.3822	2	4	5	0					
1.3680	11	3	6	1					
1.3479	3	4	0	3					

Table A.9: Data set no. 26-154 from the Powder Diffraction File (Set 45)

Pattern : 26-154 ***Radiation :*** 1.540598 ***Quality :*** Indexed

$Ba(OH)_2,H_2O$

Barium Hydroxide Hydrate

Lattice: Orthorhombic

S.G.: Pbmm (51)

Mol. weight = 189.36

Volume [CD]= 172.41

Dx = 3.648

I/Icor = 3.80

a = 6.36600 ***b*** = 6.95500 ***c*** = 3.89400

a/b = 0.91531 ***c/b*** = 0.55988

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

Z = 2

GENERAL COMMENTS: p.a.-chemical, $BaCO_3$ <2%, other impurities <0.1%.
ADDITIONAL PATTERN: To replace 1-306.

*ICDD Grant-in-Aid, (1974) primary reference : Technisch Physische Dienst, Delft, The Netherlands.
*ICDD Grant-in-Aid, unit cell data : Ibid.

Radiation: Cu

Lambda: 1.54056

SS/FOM: F30= 72(0.0122,3)

Filter: Monochromator crystal

d-sp: Guinier

d (Å)	*I*	*h*	*k*	*l*
6.3700	65	1	0	0
4.7000	100	1	1	0
3.8940	40	0	0	1
3.4780	40	0	2	0
3.3220	20	1	0	1
3.0520	8	1	2	0
2.9980	55	1	1	1
2.8930	45	2	1	0
2.5940	45	0	2	1
2.4650	10	2	0	1
2.4030	35	1	2	1
2.3480	2	2	2	0
2.3230	55	2	1	1
2.1790	14	1	3	0
2.1230	8	3	0	0
2.0300	4	3	1	0
2.0110	2	2	2	1
1.9480	16	0	0	2
1.9020	16	1	3	1
1.8740	8	2	3	0
1.8630	10	3	0	1
1.8120	6	3	2	0
1.8000	12	3	1	1
1.7400	4	0	4	0
1.7000	6	0	2	2
1.6890	8	2	3	1
1.6780	2	1	4	0
1.6610	2	2	0	2
1.6420	8	3	2	1
1.6160	10	2	1	2
1.5890	2	0	4	1
1.5650	2	3	3	0
1.5520	2	4	1	0
1.5400	2	1	4	1
1.4990	2	2	2	2
1.4740	2	4	0	1
1.4520	6	1	3	2
1.4410	1	4	1	1
1.4350	2	3	0	2
1.4200	1	2	4	1
1.4050	2	3	1	2
1.3570	2	4	2	1
1.3500	2	2	3	2
1.3450	1	3	4	0
1.3260	2	3	2	2
1.2970	2	0	4	2
1.2820	2	1	5	1
1.2710	4	1	4	2
1.2520	2	5	1	0
1.2320	1	4	0	2
1.2150	2	0	2	3
1.2090	2	5	0	1
1.1930	2	5	1	1
1.1840	2	2	1	3

Table A.10: Data set no. 26-155 from the Powder Diffraction File (Set 45)

Pattern : 26-155 ***Radiation :*** 1.540598 ***Quality :*** High

$Ba(OH)_2,8H_2O$

Barium Hydroxide Hydrate

Lattice: Monoclinic

S.G.: A2/a (15)

Mol. weight = 315.47

Volume [CD]= 1008.60

Dx = 2.077

Dm = 2.180

I/Icor = 0.40

a = 11.84500 ***b*** = 9.27700 ***c*** = 9.29200

a/b = 1.27681 ***c/b*** = 1.00162

Alpha = 90.00 ***Beta*** = 98.96 ***Gamma*** = 90.00

Z = 4

UNIT CELL DATA : Manohar and Ramaseshan, Z. Kristallogr., 119 357 (1964) give S.G.= P21/n (single crystal).
GENERAL COMMENTS: Their reflections with k+1+2n+1 are all very weak. A p.a. chemical. Impurities $BaCO_3$ <2.0%, others <0.1%.
ADDITIONAL PATTERN: To replace 1-151.

*ICDD Grant-in-Aid, (1974) primary reference : Technisch Physische Dienst, Delft, The Netherlands.
*Handbook of Chemistry and Physics, optical data :

Radiation: Cu **Filter:** Monochromator crystal

Lambda: 1.54056 **d-sp:** Guinier

SS/FOM: F30=101(0.0076,3)

d (Å)	*I*	*h*	*k*	*l*	*d (Å)*	*I*	*h*	*k*	*l*
6.5200	70	0	1	1	1.8830	2	-3	4	2
5.9900	100	-1	1	1	1.8740	2	-5	3	1
5.8500	100	2	0	0	1.8450	8	-4	3	3
5.4500	75	1	1	1	1.8220	4	-1	1	5
4.6200	25	-2	1	1	1.8060	6	-1	5	1
4.5900	45	0	0	2	1.8000	4	-2	1	5
4.3100	85	1	2	0	1.7880	6	1	5	1
4.1300	30	2	1	1	1.7400	6	1	1	5
3.9190	30	-2	0	2	1.7240	2	3	2	4
3.6350	4	-2	2	0	1.7020	4	6	0	2
3.5240	30	-3	1	1	1.6690	6	-3	5	1
3.3650	20	2	0	2	1.6600	6	4	3	3
3.2620	4	0	2	2	1.6510	4	2	1	5
3.2370	45	-1	2	2	1.6290	8	3	5	1
3.1950	25	3	1	1	1.6160	4	-6	0	4
3.0560	35	1	2	2	1.5890	10	-1	5	3
2.9850	30	-3	2	0	1.5790	8	0	3	5
2.9290	14	0	3	1	1.5570	4	1	5	3
2.8760	4	-1	3	1	1.5470	4	3	1	5
2.8100	30	1	3	1	1.5380	4	1	3	5
2.7880	10	-4	1	1	1.5290	4	0	0	6
2.7710	40	-2	1	3	1.5110	6	5	3	3
2.7280	40	1	1	3	1.4950	8	-2	6	0
2.6730	35	-2	3	1					
2.6620	10	-4	0	2					
2.6510	25	-3	2	2					
2.5690	18	2	3	1					
2.5160	6	-3	1	3					
2.4740	2	4	2	0					
2.3790	14	3	2	2					
2.3190	14	0	4	0					
2.3080	10	-4	2	2					
2.2930	10	0	0	4					
2.2870	10	3	3	1					
2.2760	10	1	4	0					
2.2600	10	-2	0	4					
2.2320	14	-4	1	3					
2.1810	14	3	1	3					
2.1750	12	0	3	3					
2.1560	8	2	4	0					
2.1230	18	-4	3	1					
2.1160	6	-2	3	3					
2.0890	4	5	2	0					
2.0750	30	-1	2	4					
2.0700	30	0	4	2					
2.0630	6	-1	4	2					
2.0310	2	-2	2	4					
2.0200	12	4	3	1					
2.0100	6	-5	2	2					
1.9940	10	-3	4	0					
1.9790	6	1	2	4					
1.9680	14	2	3	3					
1.9500	6	6	0	0					
1.9330	4	-3	2	4					
1.9240	4	4	1	3					
1.9080	2	2	4	2					

Table A.11: Data set no. 26-180 from the Powder Diffraction File (Set 45)

Pattern : 26-180 ***Radiation :*** 1.540560 ***Quality :*** High

Ba_3SiO_5

Barium Silicate

Lattice: Tetragonal

S.G.: 14/mcm (140)

Mol. weight = 520.07

Volume [CD] = 599.46

Dx = 5.763

I/Icor = 2.40

a = 7.30680 ***b*** = 7.30680 ***c*** = 11.22800

a/b = 1.00000 ***c/b*** = 1.53665

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

Z= 4

COLOR: Colorless
SAMPLE PREPARATION: Sample made by repeated grindings and heating at about 1400 °C of a 3:1 molar mixture of $BaCO_3$ and silica gel.
GENERAL COMMENTS: Pattern at 25 °C.
ADDITIONAL PATTERN: To replace 19-175 and 23-1027.

*Natl. Burl Stand. (U.S.) Monogr. 25, volume 13, page 15, (1976) primary reference:
*Natl. Burl Stand. (U.S.) Monogr. 25, unit cell data:
Ibid.
*Natl. Burl Stand. (U.S.) Monogr. 25, optical data:
Ibid.

Radiation: Cu
Lambda: 1.54056
SS/FOM: F30= 91(0.0085,3)

Filter: Monochromator crystal
d-sp: Not given
Internal standard: W

d (Å)	*I*	*h*	*k*	*l*	*d (Å)*	*I*	*h*	*k*	*l*
5.6190	7	0	0	2	1.1129	2	4	0	8
5.1690	4	1	1	0	1.0916	1	5	4	3
3.8020	20	1	1	2	1.0802	1	4	3	7
3.1380	55	2	1	1	1.0732	3	2	0	10
3.0620	100	2	0	2	1.0646	3	4	2	8
2.8080	25	0	0	4	1.0591	2	6	1	5
2.5840	30	2	2	0	1.0412	2	5	3	6
2.4620	60	2	1	3	1.0335	1	7	1	0
2.3110	30	3	1	0	1.0201	4	4	1	9
1.9940	41	3	2	1	1.0174	3	5	4	5
1.9010	20	2	2	4	1.0163	5	5	5	2
1.8720	2	0	0	6	0.9997	2	7	2	1
1.8510	12	2	1	5	0.9972	4	6	4	2
1.8270	1	4	0	0	0.9830	5	6	2	6
1.7840	16	3	1	4	0.9742	1	2	1	11
1.7600	7	1	1	6	0.9695	3	7	2	3
1.7510	20	4	1	1	0.9615	2	6	1	7
1.7380	5	4	0	2	0.9565	1	4	0	10
1.7224	2	3	3	0	0.9530	2	6	4	4
1.6657	14	2	0	6	0.9504	1	4	4	8
1.6465	16	3	3	2	0.9457	2	7	3	2
1.6338	6	4	2	0	0.9405	2	3	3	10
1.6018	6	4	1	3	0.9347	6	5	3	8
1.5687	4	4	2	2					
1.5311	3	4	0	4					
1.5041	1	3	2	5					
1.4676	1	3	3	4					
1.4492	1	4	3	1					
1.4402	4	2	1	7					
1.4120	6	4	2	4					
1.4034	3	0	0	8					
1.3912	1	4	1	5					
1.3881	10	5	1	2					
1.3614	1	4	3	3					
1.3473	1	5	2	1					
1.3074	3	4	0	6					
1.2917	2	4	4	0					
1.2757	2	5	2	3					
1.2677	6	3	3	6					
1.2584	2	4	4	2					
1.2534	5	5	3	0					
1.2335	4	2	2	8					
1.2307	3	4	2	6					
1.2231	3	5	3	2					
1.2179	4	6	0	0					
1.1994	3	3	1	8					
1.1944	3	6	1	1					
1.1892	5	4	1	7					
1.1737	1	4	4	4					
1.1655	3	2	1	9					
1.1615	2	5	2	5					
1.1442	8	5	3	4					
1.1376	2	5	1	6					
1.1350	2	5	4	1					
1.1317	6	6	2	2					
1.1172	5	6	0	4					

Table A.12: Data set no. 33-153 from the Powder Diffraction File (Set 45)

Pattern : 33-153 ***Radiation :*** 1.540598 ***Quality :*** Indexed

$Ba(OH)_2,3H_2O$

Barium Hydroxide Hydrate

Lattice: Orthorhombic

S.G.: Pnna (52)

Mol. weight = 225.39

Volume [CD]= 519.61

Dx = 0.720

a = 7.64000 ***b*** = 11.40000 ***c*** = 5.96600

a/b = 0.67018 ***c/b*** = 0.52333

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

GENERAL COMMENTS: Reference suggests space group could also be Pnnm (58).
ADDITIONAL PATTERN: To replace 21-74.

*Russ. J. Inorg. Chem. (Engl. Transl.), volume 25, page 1100, (1980) primary reference : Leshchenko, P. et al.

Radiation: CuKα1

Lambda: 1.54180

SS/FOM: F30= 57(0.0152,3)

Filter: Monochromator crystal

d-sp: Guinier

d (Å)	*I*	*h*	*k*	*l*
5.7100	60	0	2	0
5.2850	35	0	1	1
4.7010	70	1	0	1
4.3450	18	1	1	1
3.8210	40	2	0	0
3.6270	100	1	2	1
3.6270	100	2	1	0
3.2060	18	0	3	1
3.1750	40	2	2	0
3.0970	5	2	1	1
2.9820	4	0	0	2
2.9570	30	1	3	1
2.8500	18	0	4	0
2.8010	15	2	2	1
2.7010	60	1	1	2
2.6440	30	0	2	2
2.5000	12	1	2	2
2.4560	40	2	3	1
2.4360	40	1	4	1
2.3500	5	2	0	2
2.3410	15	3	0	1
2.2940	35	3	1	1
2.2840	18	2	4	0
2.2420	40	1	3	2
2.1730	15	2	2	2
2.1650	12	3	2	1
2.1320	8	2	4	1
2.1320	8	0	5	1
2.0600	12	0	4	2

Table A.13: Data set no. 43-1484 from the Powder Diffraction File (Set 45)

Pattern : 43-1484 ***Radiation :*** 1.540560 ***Quality :*** Calculated

Al_2O_3

Corundum, syn / Aluminium Oxide

Lattice: Rhombohedral

S.G.: R-3c (167)

Mol. weight = 101.96

Volume [CDT] = 254.84

Dx = 3.986

I/Icor = 0.98

a = 4.75920 ***b*** = 4.75920 ***c*** = 12.99200

a/b = 1.00000 ***c/b*** = 2.72987

Alpha = 90.00 ***Beta*** = 90.00 ***Gamma*** = 90.00

Z= 6

GENERAL COMMENTS: Calculation of diffractometer peak intensities done with MICRO-POWD v.2.2 (D. Smith and K. Smith) using default instrument broadening function (NBS Table), diffracted beam monochromator polarization correction, and atomic scattering factors corrected for anomalous dispersion. Cell parameters from D. Smith documentation for MICRO-POWD sample file (original structure data after Newnham and De Haan). Atomic positions from same source: Al in 12c with z=0.352, O in 18e with x=0.306. Isotropic thermal parameters also from Smith: Al, B=0.14; O, B=0.22.

*ICDD Grant-in-Aid, (1991) primary reference:
Grier, D., McCarthy, G., North Dakota State University, Fargo, North Dakota, USA.
*Acta Crystallogr., Sec. A, volume 46, page 271, (1990):

Radiation: CuKα1

Lambda: 1.54056

SS/FOM: F30=416(0.0024,3)

Filter: Monochromator crystal

d-sp: Calculated spacings

No standard

d (Å)	*I*	*h*	*k*	*l*
3.4800	72	0	1	2
2.5510	98	1	0	4
2.3800	44	1	1	0
2.1650	1	0	0	6
2.0860	100	1	1	3
1.9643	2	2	0	2
1.7401	48	0	2	4
1.6015	96	1	1	6
1.5467	3	2	1	1
1.5149	4	1	2	2
1.5109	9	0	1	8
1.4046	38	2	1	4
1.3739	57	3	0	0
1.3361	1	1	2	5
1.2755	1	2	0	8
1.2391	17	1	0	10
1.2342	10	1	1	9
1.1932	1	2	1	7
1.1898	7	2	2	0
1.1601	1	3	0	6
1.1473	5	2	2	3
1.1387	1	1	3	1
1.1258	4	3	1	2
1.1242	4	1	2	8
1.0990	8	0	2	10
1.0827	2	0	0	12
1.0783	10	1	3	4
1.0463	1	3	1	5
1.0428	19	2	2	6
1.0177	2	0	4	2
0.9978	14	2	1	10
0.9855	1	1	1	12
0.9822	3	4	0	4
0.9733	1	1	3	7
0.9431	1	3	2	1
0.9412	1	1	2	11
0.9357	1	2	3	2
0.9348	4	3	1	8
0.9181	3	2	2	9
0.9079	13	3	2	4
0.9053	10	0	1	14
0.8994	8	4	1	0

Table A.14: Data set no. 43-256 from the Powder Diffraction File (Set 45)

Pattern : 43-256 ***Radiation :*** 1.540560 ***Quality :*** High

$Ba_2Fe_2O_5$

Barium Iron Oxide

Lattice: Monoclinic

S.G.: P21/c (14)

Mol. weight = 466.35

Volume [CD] = 1892.19

Dx = 5.730

a = 6.96900 ***b*** = 11.72400 ***c*** = 23.43100

a/b = 0.59442 ***c/b*** = 1.99855

Alpha = 90.00 ***Beta*** = 98.74 ***Gamma*** = 90.00

Z= 14

COLOR: Brown
SAMPLE PREPARATION: Prepared by solid state reaction at 1100 °C in air.
GENERAL COMMENTS: Several reflections have been reindexed, better to fit the cell.

*Private Communication, (1991) primary reference: Gonzalez-Calbet, J., Universidad Complutense, Dept. Qulmica Inorganica I, Madrid, Spain.
*Mater. Res. Bull., volume 22, page 1413, (1987) powder data:
*J. Solid State Chem., volume 86, page 261, (1990) powder data:
*J. Solid State Chem., volume 80, page 6, (1989):

Radiation: CuKα
Lambda: 1.54180
SS/FOM: F30= 6(0.0148,31)

Filter: Monochromator crystal
d-sp: Diffractometer
No standard

d (Å)	*I*	*h*	*k*	*l*
10.430	4	0	1	1
4.1360	12	1	0	4
4.0440	24	1	2	-3
3.8600	1	0	3	-1
3.6660	1	0	1	-6
3.4470	3	2	0	2
3.3040	5	2	1	-2
3.2120	6	2	1	-3
3.1750	1	2	0	2
3.1700	1	1	0	6
3.0580	3	1	1	6
3.0280	3	1	3	3
2.9330	52	0	4	0
2.9070	100	0	4	1
2.8830	98	0	2	-7
2.7910	58	2	0	-6
2.6970	2	1	4	-1
2.6930	1	1	4	0
2.6510	3	1	3	-6
2.5310	3	2	1	-7
2.4610	10	1	3	6
2.3910	30	1	4	4
2.3200	14	3	0	-2
2.2980	13	0	5	2
2.2650	5	2	3	4
2.0660	35	2	0	8
2.0200	64	2	4	-6
2.0010	1	3	1	4
1.9810	3	0	2	-11
1.8460	5	3	2	5
1.8400	5	1	2	-12
1.8370	5	1	2	11
1.8210	5	0	5	8
1.8120	5	1	4	-10
1.7730	5	3	2	-9
1.6890	19	2	4	8
1.6850	17	2	6	1
1.6820	20	0	6	-7
1.6680	9	4	0	2

Table A.15: Data set no. 44-585 from the Powder Diffraction File (Set 45)

Pattern : 44-585	***Radiation :*** 1.540598	***Quality :*** Indexed	

$Ba(OH)_2$

Barium Hydroxide

Lattice: Monoclinic

S.G.: P21/* (11)

Mol. weight = 171.34

Volume [CD]= 504.16

Dx = 4.515

a = 6.78350 ***b*** = 7.92680 ***c*** = 9.42460

a/b = 0.85577 ***c/b*** = 1.18895

Alpha = 90.00 ***Beta*** = 95.82 ***Gamma*** = 90.00

Z= 8

COLOR: White
SAMPLE PREPARATION: Prepared from Ba + H_2O at 190 °C in CO_2-free environment
ADDITIONAL PATTERN: To replace 21-72 and 21-73.

CAS: 17194-00-2

*Private Communication, (1993) primary reference : van Vlaanderen, P., Energieonderzoek Centrum nederland, Petten, The Netherlands.
*J. Chem. Thermodyn., volume 20, page 989, (1988) unit cell data : Komings, R. et al.

Radiation: CuKα1

Lambda: 1.54060

SS/FOM: F30= 46(0.0105,6)

Filter: Monochromator crystal

d-sp: Guinier

Internal standard: SiO_2

d (Å)	*I*	*h*	*k*	*l*
5.7670	10	-1	0	1
5.1390	5	1	1	0
4.6690	20	-1	1	1
4.3690	10	1	1	1
4.0360	30	0	1	2
3.9650	15	0	2	0
3.6060	60	-1	1	2
3.4180	100	1	2	0
3.3760	80	2	0	0
3.3398	80	1	1	2
3.2650	50	-1	2	1
3.1580	30	1	2	1
3.0286	30	0	2	2
2.9526	60	-1	0	3
2.9080	50	0	1	3
2.8333	20	-1	2	2
2.7328	30	1	0	3
2.7090	60	-2	1	2
2.5693	40	2	2	0
2.5438	70	0	3	1
2.4831	70	2	1	2
2.4549	60	0	2	3
2.4301	5	2	2	1
2.3668	5	-1	2	3
2.3445	20	0	0	4
2.3296	10	-2	2	2
2.3012	40	0	3	2
2.2121	5	-1	3	2
2.1971	10	-1	1	4
2.1641	20	3	1	0
2.1060	20	2	1	3
2.0643	40	-2	2	3
2.0419	20	-3	1	2
2.0179	30	0	3	3
2.0179	30	0	2	4
2.0045	40	2	3	1
1.9818	20	0	4	0
1.9567	40	3	2	0
1.9476	20	-2	3-	2
1.9385	30	0	4	1
1.9203	30	-3	0	3

APPENDIX B

TABLED VALUES OF THE RATIO OF DIBARIUM SILICATE TO BARIUM CARBONATE IN THE QUATERNARY SAMPLES

The peaks at $2\theta = 29.585°$ and $2\theta = 23.901°$ in the diffractograms of the quaternary samples are almost solely due to the reflections of dibarium silicate and barium carbonate, respectively. In Tables B.1 to B.5, the ratios of these two peak intensities in the different diffractograms are given, as discussed in Chapter 4.

Table B.1: Ratios of the peak intensity at $2\theta = 29.585°$ and $2\theta = 23.901°$ in the diffractograms of the quaternary samples with BSF = 86 %

Heating Time (minutes)	Ratio at Different Heating Temperatures				
	1000 °C	1100 °C	1200 °C	1300 °C	1400 °C
15	0.420	0.553	0.990	5.032	10.916
30	0.532	0.864	1.620	1.723	5.226
60	0.596	1.291	1.572	13.498	5.053
120	0.817	1.198	3.282	4.077	2.855

Table B.2: Ratios of the peak intensity at $2\theta = 29.585°$ and $2\theta = 23.901°$ in the diffractograms of the quaternary samples with BSF = 90 %

Heating Time (minutes)	Ratio at Different Heating Temperatures				
	1000 °C	1100 °C	1200 °C	1300 °C	1400 °C
15	0.424	0.535	0.824	5.040	18.504
30	0.338	0.680	1.253	3.790	7.240
60	0.627	0.915	1.737	1.922	9.364
120	0.798	1.823	2.472	3.051	11.127

Table B.3: Ratios of the peak intensity at 2θ = 29.585° and 2θ = 23.901° in the diffractograms of the quaternary samples with BSF = 94 %

Heating Time (minutes)	Ratio at Different Heating Temperatures				
	1000 °C	1100 °C	1200 °C	1300 °C	1400 °C
15	0.423	0.536	0.697	2.334	2.884
30	0.384	0.686	0.897	2.470	4.324
60	0.491	0.990	2.141	3.501	6.080
120	0.617	1.353	1.623	3.205	2.299

Table B.4: Ratios of the peak intensity at 2θ = 29.585° and 2θ = 23.901° in the diffractograms of the quaternary samples with BSF = 98 %

Heating Time (minutes)	Ratio at Different Heating Temperatures				
	1000 °C	1100 °C	1200 °C	1300 °C	1400 °C
15	0.283	0.535	0.672	2.432	3.418
30	0.420	0.638	0.593	2.509	2.588
60	0.502	0.848	0.822	2.572	2.954
120	0.596	0.540	5.020	1.551	2.995

Table B.5: Ratios of the peak intensity at 2θ = 29.585° and 2θ = 23.901° in the diffractograms of the quaternary samples with BSF = 102 %

Heating Time (minutes)	Ratio at Different Heating Temperatures				
	1000 °C	1100 °C	1200 °C	1300 °C	1400 °C
15	0.346	0.488	0.640	2.703	4.008
30	0.304	0.473	0.707	2.999	2.482
60	0.412	0.666	1.313	2.832	1.602
120	0.570	0.750	1.433	2.549	1.982