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# LAMPIRAN

Sampel BT1



Sampel BT2



Sampel BT3



Sampel BT4



Sampel BT5



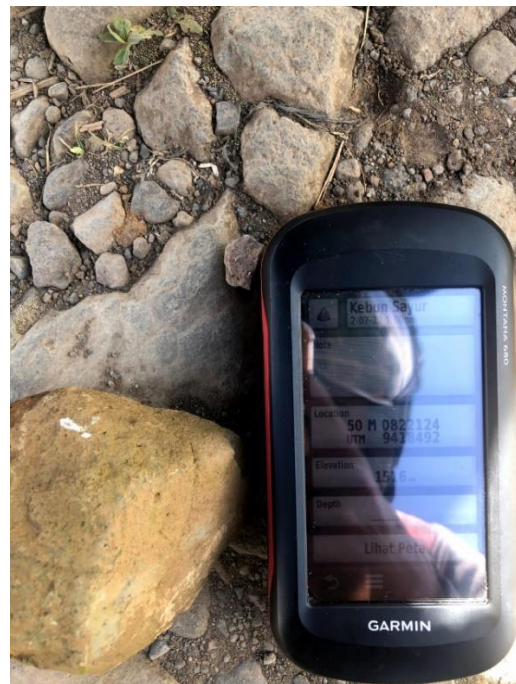
Sampel Jembatan Merah



Sampel Jalan Lembanna



Sampel Kebun Lembanna



Sampel Pos 1.1 Bawakaraeng



Sampel Pos 1 Bawakaraeng



Sampel Takapala



# HASIL XRD

## Match! Phase Analysis Report

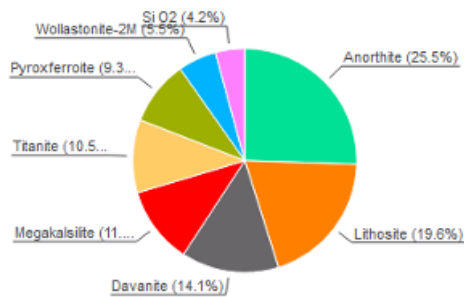
Sample: TEST SAMPLE

### Sample Data

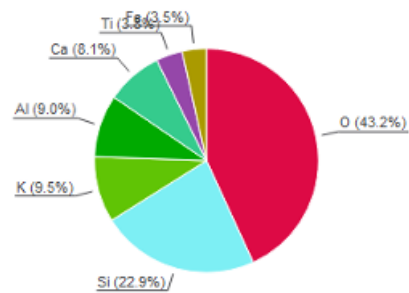
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 File path: C:/Users/AGUNGP~1/AppData/Local/Temp/Rar\$DRa11372.9016/Hasil XRD  
 Data collected: Agu 22, 2022 05:52:07  
 Data range: 10.300° - 90.300°  
 Original data range: 10.000° - 90.000°  
 Number of points: 4001  
 Step size: 0.020  
 Rietveld refinement converged: No  
 Alpha2 subtracted: No  
 Background subtr.: No  
 Data smoothed: Yes  
 2theta correction: 0.3°  
 Radiation: X-rays  
 Wavelength: 1.540598 Å

### Analysis Results

Phase composition (Weight %)



Elemental composition (Weight %)



Index	Amount (%)	Name	Formula sum
A	25.5	Anorthite	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
B	19.6	Lithosite	Al <sub>2</sub> K <sub>3</sub> O <sub>13</sub> Si <sub>4</sub>
C	14.1	Davanite	K <sub>2</sub> O <sub>15</sub> Si <sub>8</sub> Ti
D	11.2	Megakalsilite	Al K O <sub>4</sub> Si
E	10.5	Titanite	Ca O <sub>5</sub> Si Ti
F	9.3	Pyroxferroite	Ca <sub>0.94</sub> Fe <sub>0.06</sub> O <sub>21</sub> Si <sub>7</sub>
G	5.5	Wollastonite-2M	Ca O <sub>3</sub> Si
H	4.2	Si O <sub>2</sub>	O <sub>2</sub> Si
	1.4	Unidentified peak area	

Element	Amount (weight %)
O	43.2% (*)
Si	22.9%
K	9.5%
Al	9.0%
Ca	8.1%
Ti	3.8%
Fe	3.5%
*LE (sum)	43.2%

Amounts calculated by RIR (Reference Intensity Ratio) method

### Details of identified phases

**A: Anorthite (25.5 %)**  
 Formula sum: Al<sub>2</sub> Ca O<sub>8</sub> Si<sub>2</sub>  
 Entry number: 96-900-0363  
 Figure-of-Merit (FoM): 0.852919  
 Total number of peaks: 500  
 Peaks in range: 500



Unit cell	a= 8.2230 Å b= 12.9150 Å c= 14.2040 Å $\alpha$ = 92.750° $\beta$ = 115.800° $\gamma$ = 91.020°
I/lc	0.51
Calc. density	2.727 g/cm <sup>3</sup>
Reference	Foit F. F., Peacor D. R., "The anorthite crystal structure at 410 and 830 CT = 830 C", American Mineralogist 58, 665-675 (1973)
<b>B: Lithosite (19.6 %)</b> <sup>*</sup>	
Formula sum	Al <sub>2</sub> K <sub>3</sub> O <sub>13</sub> Si <sub>4</sub>
Entry number	96-901-1908
Figure-of-Merit (FoM)	0.847830 <sup>*</sup>
Total number of peaks	499
Peaks in range	499
Peaks matched	498
Intensity scale factor	0.31 <sup>*</sup>
Space group	P 1 2 1 1
Crystal system	monoclinic
Unit cell	a= 15.1970 Å b= 10.2330 Å c= 8.4350 Å $\beta$ = 90.310°
I/lc	0.60
Calc. density	2.489 g/cm <sup>3</sup>
Reference	Pudovkina Z. V., Solov'eva L. P., Pyatenko Y. A., "Crystal structure of lithosite K <sub>3</sub> [HAl <sub>2</sub> Si <sub>4</sub> O <sub>13</sub> ]", Soviet Physics Doklady 31, 941-942 (1986)
<b>C: Davanite (14.1 %)</b> <sup>*</sup>	
Formula sum	K <sub>2</sub> O <sub>15</sub> Si <sub>8</sub> Ti
Entry number	96-900-9617
Figure-of-Merit (FoM)	0.823978
Total number of peaks	500
Peaks in range	500
Peaks matched	500
Intensity scale factor	0.27 <sup>*</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 7.2500 Å b= 7.4740 Å c= 6.9090 Å $\alpha$ = 105.590° $\beta$ = 112.810° $\gamma$ = 99.280°
I/lc	0.71
Calc. density	2.799 g/cm <sup>3</sup>
Reference	Gebert W., Medenbach O., Florke O. W., "Darstellung und kristallographie von K <sub>2</sub> TiSi <sub>8</sub> O <sub>15</sub> - isotyp mit dalyitK <sub>2</sub> ZrSi <sub>8</sub> O <sub>15</sub> Locality: synthetic", Tschermaks Mineralogische und Petrographische Mitteilungen 31, 69-79 (1983)
<b>D: Megakalsilite (11.2 %)</b> <sup>*</sup>	
Formula sum	Al K O <sub>4</sub> Si
Entry number	96-900-4886
Figure-of-Merit (FoM)	0.858024 <sup>*</sup>
Total number of peaks	290
Peaks in range	290
Peaks matched	288
Intensity scale factor	0.62 <sup>*</sup>
Space group	P 63
Crystal system	hexagonal
Unit cell	a= 18.1111 Å c= 8.4619 Å
I/lc	2.07
Calc. density	2.622 g/cm <sup>3</sup>
Reference	Khomyakov A. P., Nechelyustov G. N., Sokolova E. V., Bonaccorsi E., Merlino S., Pasero M., "Megakalsilite, a new polymorph of KAlSi <sub>4</sub> O <sub>8</sub> from the Khibina alkaline massif, Kola Peninsula, Russia: mineral description and crystal structure", The Canadian Mineralogist 40, 961-970 (2002)
<b>E: Titanite (10.5 %)</b> <sup>*</sup>	
Formula sum	Ca O <sub>5</sub> Si Ti
Entry number	96-900-2464
Figure-of-Merit (FoM)	0.786205 <sup>*</sup>
Total number of peaks	286
Peaks in range	144
Peaks matched	144
Intensity scale factor	0.37 <sup>*</sup>
Space group	A 1 2/a 1
Crystal system	monoclinic
Unit cell	a= 6.9409 Å b= 8.6532 Å c= 6.4551 Å $\beta$ = 113.331°
I/lc	1.30
Calc. density	3.658 g/cm <sup>3</sup>
Reference	Kunz M., Arlt T., Stolz J., "In situ powder diffraction study of titanite (CaTiOSiO <sub>4</sub> ) at high pressure and high temperature Sample", American Mineralogist 85, 1465-1473 (2000)
<b>F: Pyroxferroite (9.3 %)</b>	
Formula sum	Ca <sub>0.94</sub> Fe <sub>0.06</sub> O <sub>21</sub> Si <sub>7</sub>
Entry number	96-901-2890
Figure-of-Merit (FoM)	0.820814
Total number of peaks	496
Peaks in range	496

Peaks matched 495  
 Intensity scale factor 0.22  
 Space group P-1  
 Crystal system triclinic (anorthic)  
 Unit cell a= 6.6213 Å b= 7.5506 Å c= 17.3806 Å  $\alpha$ = 114.267°  $\beta$ = 82.884°  $\gamma$ = 94.576°  
 Ilc 0.89  
 Calc. density 3.843 g/cm<sup>3</sup>  
 Reference Burnham C. W., "The crystal structure of pyroxferroite from Mare Tranquillitatis", Proceedings of the Second Lunar Science Conference 1, 47-57 (1971)

**G: Wollastonite-2M (5.5 %)**

Formula sum Ca O3 Si  
 Entry number 96-901-1453  
 Figure-of-Merit (FoM) 0.834180  
 Total number of peaks 498  
 Peaks in range 498  
 Peaks matched 498  
 Intensity scale factor 0.26  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 15.4090 Å b= 7.3220 Å c= 7.0630 Å  $\beta$ = 95.300°  
 Ilc 1.75  
 Calc. density 2.917 g/cm<sup>3</sup>  
 Reference Hesse K.-F., "Refinement of the crystal structure of wollastonite-2M (parawollastonite)", Zeitschrift für Kristallographie 168, 93-98 (1984)

**H: Si O2 (4.2 %)**

Formula sum O2 Si  
 Entry number 96-412-4066  
 Figure-of-Merit (FoM) 0.814152  
 Total number of peaks 491  
 Peaks in range 490  
 Peaks matched 490  
 Intensity scale factor 0.17  
 Space group P b c a  
 Crystal system orthorhombic  
 Unit cell a= 8.7724 Å b= 8.7833 Å c= 16.1865 Å  
 Ilc 1.51  
 Calc. density 2.559 g/cm<sup>3</sup>  
 Reference Foster M.D., Friedrichs O.D., Bell R.G., Paz F.A.A., Klinowski J., "Chemical evaluation of hypothetical uninodal zeolites", Journal of the American Chemical Society 126, 9769-9775 (2004)

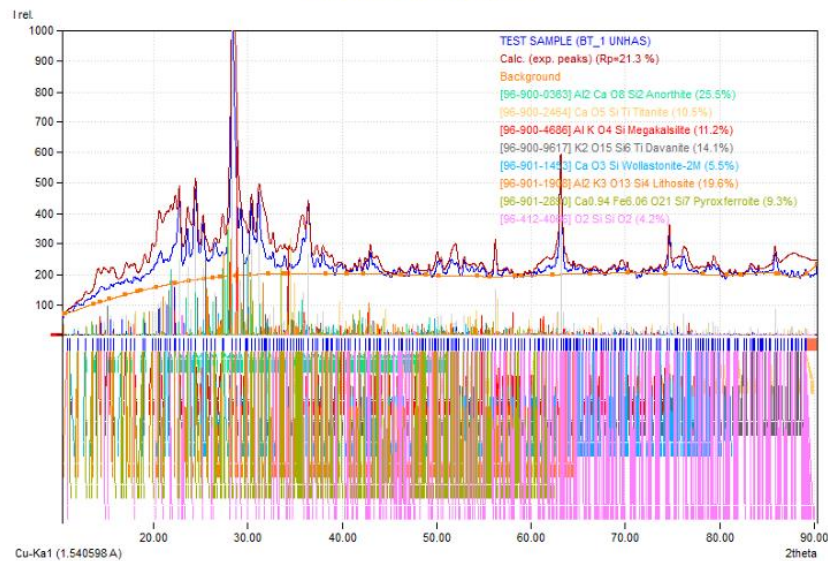
[<sup>†</sup>] 2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

Profile area	Counts	Amount
Overall diffraction profile	660132	100.00%
Background radiation	540878	81.93%
Diffraction peaks	119253	18.07%
Peak area belonging to selected phases	110336	16.71%
Peak area of phase A (Anorthite)	23766	3.60%
Peak area of phase B (Titanite)	11565	1.75%
Peak area of phase C (Megakalsilite)	12012	1.82%
Peak area of phase D (Davanite)	18623	2.82%
Peak area of phase E (Wollastonite-2M)	7720	1.17%
Peak area of phase F (Lithosite)	19303	2.92%
Peak area of phase G (Pyroxferroite)	10506	1.59%
Peak area of phase H (Si O2)	6842	1.04%
Unidentified peak area	8917	1.35%

**Peak Residuals**

Peak data	Counts	Amount
Overall peak intensity	4315	100.00%
Peak intensity belonging to selected phases	3992	92.51%
Unidentified peak intensity	323	7.49%

**Diffraction Pattern Graphics**



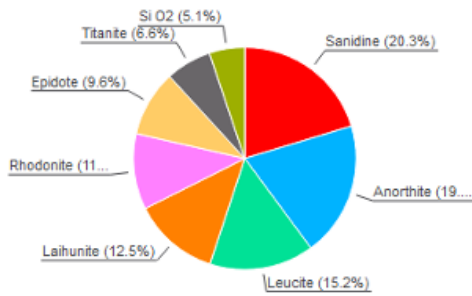
Sample: TEST SAMPLE

Sample Data

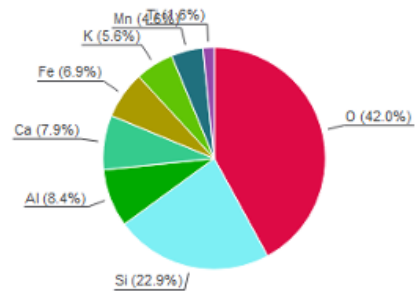
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 Original data range 10.000° - 90.000°  
 Number of points 4001  
 Step size 0.020  
 Rietveld refinement converged No  
 Alpha2 subtracted No  
 Background subtr. No  
 Data smoothed Yes  
 2theta correction -0.08°  
 Radiation X-rays  
 Wavelength 1.540598 Å

Analysis Results

Phase composition (Weight %)



Elemental composition (Weight %)



Index	Amount (%)	Name	Formula sum
A	20.3	Sanidine	Al K O8 Si3
B	19.6	Anorthite	Al Ca O4 Si
C	15.2	Leucite	Al K O6 Si2
D	12.5	Laihunite	Fe4.74 O12 Si3
E	11.0	Rhodonite	Mn5 O15 Si5
F	9.6	Epidote	Al2.32 Ca2 Fe0.68 O13 Si3
G	6.6	Titanite	Ca O5 Si Ti
H	5.1	Si O2	O2 Si
	2.8	Unidentified peak area	

Element	Amount (weight %)
O	42.0% (*)
Si	22.9%
Al	8.4%
Ca	7.9%
Fe	6.9%
K	5.6%
Mn	4.6%
Ti	1.6%
*LE (sum)	42.0%

Amounts calculated by RIR (Reference Intensity Ratio) method

Details of identified phases

**A: Sanidine (20.3 %)**  
 Formula sum Al K O8 Si3  
 Entry number 96-900-4247  
 Figure-of-Merit (FoM) 0.847292  
 Total number of peaks 292  
 Peaks in range 292  
 Peaks matched 292  
 Intensity scale factor 0.37  
 Space group C 1 2/m 1  
 Crystal system monoclinic

Unit cell	a= 8.6110 Å b= 13.0460 Å c= 7.1750 Å β= 116.010 °
I/lc	0.73
Calc. density	2.552 g/cm <sup>3</sup>
Reference	Ferguson R. B., Ball N. A., Cerny P., "Structure refinement of an adularian end-member high sanidine from the Buck Claim Pegmatite, Bernic Lake, Manitoba Sample: III Note: variety adularia", The Canadian Mineralogist 29, 543-552 (1991)
<b>B: Anorthite (19.6 %)<sup>+</sup></b>	
Formula sum	Al Ca O4 Si
Entry number	96-900-1262
Figure-of-Merit (FoM)	0.824217
Total number of peaks	248
Peaks in range	248
Peaks matched	247
Intensity scale factor	0.29 <sup>+</sup>
Space group	I -1
Crystal system	triclinic (anorthic)
Unit cell	a= 8.1780 Å b= 12.8700 Å c= 14.1750 Å α= 93.170° β= 115.970 ° γ= 91.150 °
I/lc	0.59
Calc. density	3.161 g/cm <sup>3</sup>
Reference	Angel R. J., Carpenter M. A., Finger L. W., "Structural variation associated with compositional variation and order-disorder behavior in anorthite-rich feldspars sample", American Mineralogist 75, 150-162 (1990)
<b>C: Leucite (15.2 %)<sup>+</sup></b>	
Formula sum	Al K O6 Si2
Entry number	96-900-1796
Figure-of-Merit (FoM)	0.837608 <sup>+</sup>
Total number of peaks	141
Peaks in range	141
Peaks matched	140
Intensity scale factor	0.52 <sup>+</sup>
Space group	I 41/a
Crystal system	tetragonal
Unit cell	a= 13.0548 Å c= 13.7518 Å
I/lc	1.38
Calc. density	2.474 g/cm <sup>3</sup>
Reference	Palmer D. C., Dove M. T., Ibberson R. M., Powell B. M., "Structural behavior, crystal chemistry and phase transitions in substituted leucites: High-resolution neutron powder diffraction studies Sample: Natural, Expt. no. 3003, T = 298 K, KAlSi2O6", American Mineralogist 82, 16-29 (1997)
<b>D: Laihunite (12.5 %)<sup>+</sup></b>	
Formula sum	Fe4.74 O12 Si3
Entry number	96-900-1036
Figure-of-Merit (FoM)	0.859302 <sup>+</sup>
Total number of peaks	497
Peaks in range	497
Peaks matched	496
Intensity scale factor	0.43 <sup>+</sup>
Space group	P 21/b 1 1
Crystal system	monoclinic
Unit cell	a= 4.8050 Å b= 10.1890 Å c= 17.4030 Å α= 91.000°
I/lc	1.40
Calc. density	4.218 g/cm <sup>3</sup>
Reference	Shen B., Tamada O., Kitamura M., Morimoto N., "Superstructure of laihunite-3M (Fe4.74O12Si3) Sample: Superstructure Fe1B-y coordinate changed by Tamada (Aug, 2001)", American Mineralogist 71, 1455-1460 (1986)
<b>E: Rhodonite (11.0 %)<sup>+</sup></b>	
Formula sum	Mn5 O15 Si5
Entry number	96-900-3679
Figure-of-Merit (FoM)	0.805724 <sup>+</sup>
Total number of peaks	246
Peaks in range	246
Peaks matched	244
Intensity scale factor	0.26 <sup>+</sup>
Space group	C -1
Crystal system	triclinic (anorthic)
Unit cell	a= 9.7999 Å b= 10.5176 Å c= 12.2365 Å α= 108.587° β= 103.185 ° γ= 82.320 °
I/lc	0.96
Calc. density	3.747 g/cm <sup>3</sup>
Reference	Nelson W. R., Griffen D. T., "Crystal chemistry of Zn-rich rhodonite ("fowlerite") Sample: 15-4025 Note: see samples 15-4029 and 15-4024 for plausible typical fowlerite and rhodonite cation distributions", American Mineralogist 90, 969-983 (2005)
<b>F: Epidote (9.6 %)<sup>+</sup></b>	
Formula sum	Al2.32 Ca2 Fe0.68 O13 Si3
Entry number	96-900-2181
Figure-of-Merit (FoM)	

0.785046<sup>†</sup>  
 Total number of peaks 499  
 Peaks in range 427  
 Peaks matched 421  
 Intensity scale factor 0.20<sup>†</sup>  
 Space group P 1 21/m 1  
 Crystal system monoclinic  
 Unit cell a= 8.8910 Å b= 5.6240 Å c= 10.1640 Å β= 115.440 °  
 I/lc 0.82  
 Calc. density 3.423 g/cm<sup>3</sup>  
 Reference Giuli G., Bonazzi P., Menchetti S., "Al-Fe disorder in synthetic epidotes: A single-crystal X-ray diffraction study Sample: CC11c", American Mineralogist 84, 933-936 (1999)

**G: Titanite (6.6 %)<sup>†</sup>**  
 Formula sum Ca O5 Si Ti  
 Entry number 96-900-0511  
 Figure-of-Merit (FoM) 0.815109<sup>†</sup>  
 Total number of peaks 500  
 Peaks in range 300  
 Peaks matched 295  
 Intensity scale factor 0.24<sup>†</sup>  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 7.0670 Å b= 8.7260 Å c= 6.5680 Å β= 113.770 °  
 I/lc 1.47  
 Calc. density 3.513 g/cm<sup>3</sup>  
 Reference Taylor M., Brown G. E., "High-temperature structural study of the P2<sub>1</sub>/a - A2/a phase transition in synthetic titanite, CaTiSiO<sub>5</sub> = 165 deg C", American Mineralogist 61, 435-447 (1976)

**H: Si O2 (5.1 %)<sup>†</sup>**  
 Formula sum O2 Si  
 Entry number 96-412-4049  
 Figure-of-Merit (FoM) 0.808802<sup>†</sup>  
 Total number of peaks 130  
 Peaks in range 130  
 Peaks matched 130  
 Intensity scale factor 0.46<sup>†</sup>  
 Space group F d d d  
 Crystal system orthorhombic  
 Unit cell a= 4.8424 Å b= 15.1161 Å c= 20.6075 Å  
 I/lc 3.61  
 Calc. density 2.116 g/cm<sup>3</sup>  
 Reference Foster M.D., Bell R.G., Friedrichs O.D., Paz F.A.A., Klinowski J., "Chemical evaluation of hypothetical uninodal zeolites", Journal of the American Chemical Society 126, 9769-9775 (2004)

<sup>†</sup>2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

### Integrated Profile Areas

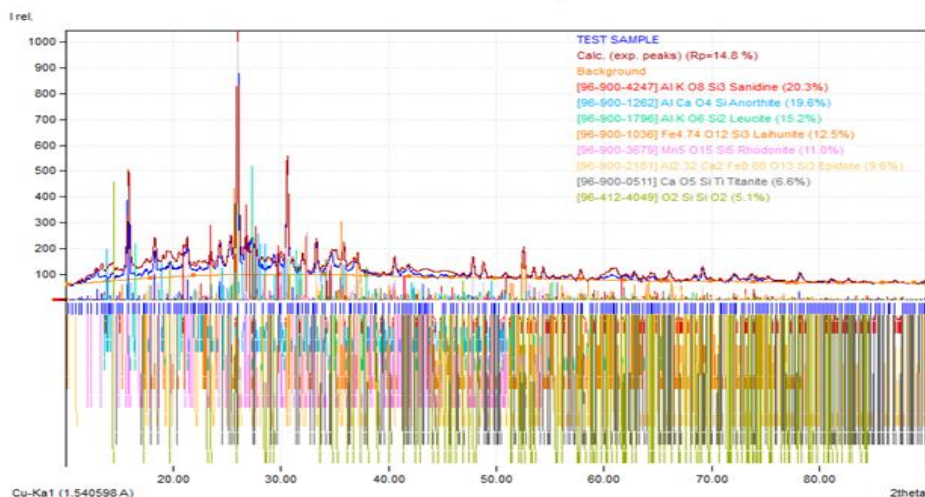
Based on calculated profile

Profile area	Counts	Amount
Overall diffraction profile	1059208	100.00%
Background radiation	816066	77.04%
Diffraction peaks	243142	22.96%
Peak area belonging to selected phases	213436	20.15%
Peak area of phase A (Sanidine)	44976	4.25%
Peak area of phase B (Anorthite)	39433	3.72%
Peak area of phase C (Leucite)	28904	2.73%
Peak area of phase D (Laihunite)	32123	3.03%
Peak area of phase E (Rhodonite)	18823	1.78%
Peak area of phase F (Epidote)	20849	1.97%
Peak area of phase G (Titanite)	14061	1.33%
Peak area of phase H (Si O2)	14267	1.35%
Unidentified peak area	29706	2.80%

### Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	6895	100.00%
Peak intensity belonging to selected phases	6571	95.30%
Unidentified peak intensity	324	4.70%

### Diffraction Pattern Graphics



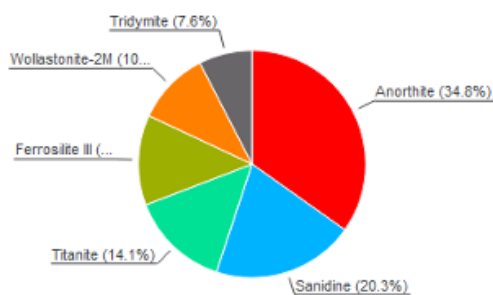
## Sample: TEST SAMPLE

### Sample Data

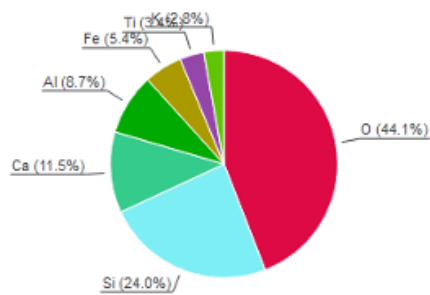
File name	BT_3 UNHAS.raw
File path	C:/Users/AGUNGP~1/AppData/Local/Temp/Rar\$DRa11372.26093/Hasil XRD
Data collected	Agu 18, 2022 06:00:12
Data range	9.780° - 89.780°
Original data range	10.000° - 90.000°
Number of points	4001
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	-0.22°
Radiation	X-rays
Wavelength	1.540598 Å

### Analysis Results

**Phase composition (Weight %)**



**Elemental composition (Weight %)**



#### Index Amount (%) Name

A	34.8	Anorthite	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
B	20.3	Sanidine	Al K O <sub>8</sub> Si <sub>3</sub>
C	14.1	Titanite	Ca O <sub>5</sub> Si Ti
D	12.8	Ferrosilite III	Fe O <sub>3</sub> Si
E	10.5	Wollastonite-2M	Ca O <sub>3</sub> Si
F	7.6	Tridymite	O <sub>2</sub> Si
	0.4	Unidentified peak area	

#### Element Amount (weight %)

O	44.1% (*)
Si	24.0%
Ca	11.5%
Al	8.7%
Fe	5.4%
Ti	3.4%
K	2.8%
*LE (sum)	44.1%

Amounts calculated by RIR (Reference Intensity Ratio) method

#### Details of identified phases

##### A: Anorthite (34.8 %)\*

Formula sum	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
Entry number	96-900-0363
Figure-of-Merit (FoM)	0.856940
Total number of peaks	500
Peaks in range	500
Peaks matched	497
Intensity scale factor	0.41 <sup>†</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 8.2230 Å b= 12.9150 Å c= 14.2040 Å α= 92.750° β= 115.800° γ= 91.020°
I/Ic	0.51
Calc. density	2.727 g/cm <sup>3</sup>

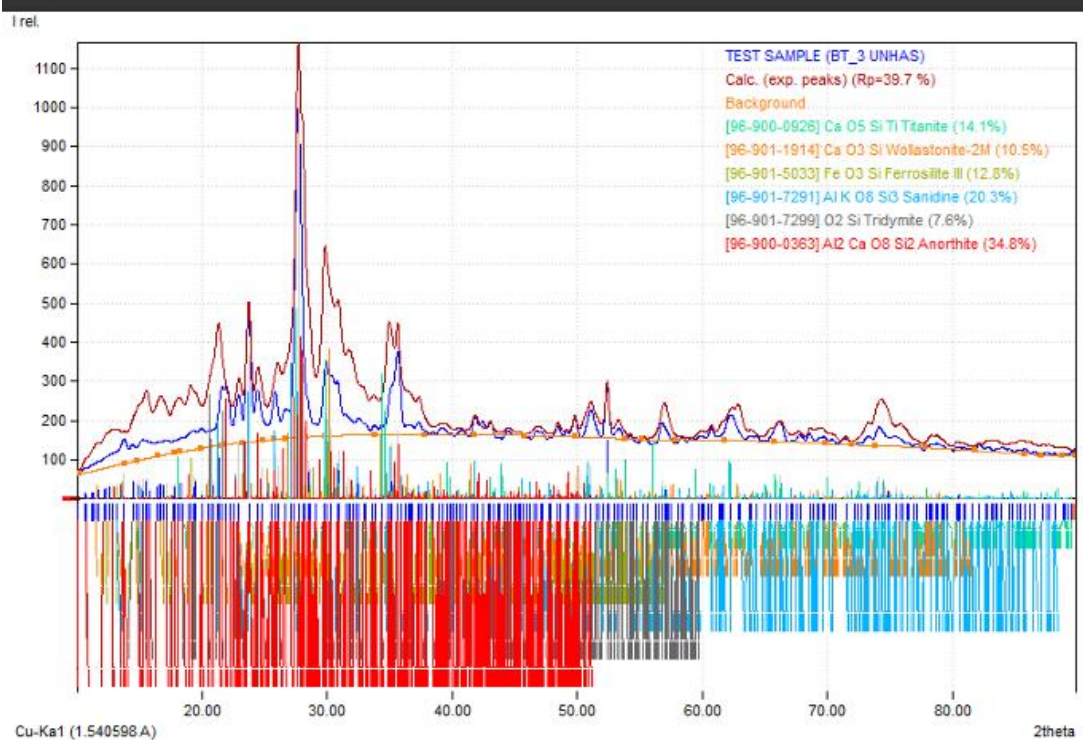
Reference	Foit F. F., Peacor D. R., "The anorthite crystal structure at 410 and 830 °C = 830 °C", <i>American Mineralogist</i> <b>58</b> , 665-675 (1973)
<b>B: Sanidine (20.3 %)*</b>	
Formula sum	Al K O8 Si3
Entry number	98-901-7291
Figure-of-Merit (FoM)	0.819263 <sup>†</sup>
Total number of peaks	293
Peaks in range	293
Peaks matched	293
Intensity scale factor	0.35 <sup>†</sup>
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 8.4800 Å b= 12.9700 Å c= 7.1800 Å β= 115.980 °
I/Ic	0.74
Calc. density	2.604 g/cm <sup>3</sup>
Reference	Ribbe P. H., "A refinement of the crystal structure of sanidinised orthoclase Note: Occupancies not provided, estimated using Kroll & Ribbe, 1983", <i>Acta Crystallographica</i> <b>16</b> , 426-427 (1983)
<b>C: Titanite (14.1 %)*</b>	
Formula sum	Ca O5 Si Ti
Entry number	98-900-0926
Figure-of-Merit (FoM)	0.833178 <sup>†</sup>
Total number of peaks	500
Peaks in range	323
Peaks matched	319
Intensity scale factor	0.49 <sup>†</sup>
Space group	P 1 2 1 1
Crystal system	monoclinic
Unit cell	a= 7.0500 Å b= 8.6810 Å c= 6.5390 Å β= 113.900 °
I/Ic	1.48
Calc. density	3.559 g/cm <sup>3</sup>
Reference	Hollabaugh C. L., Foit F. F., "The crystal structure of an Al-rich titanite from Grisons, Switzerland", <i>American Mineralogist</i> <b>69</b> , 725-732 (1984)
<b>D: Ferrosilite III (12.8 %)*</b>	
Formula sum	Fe O3 Si
Entry number	98-901-5033
Figure-of-Merit (FoM)	0.798624 <sup>†</sup>
Total number of peaks	499
Peaks in range	499
Peaks matched	497
Intensity scale factor	0.16 <sup>†</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 6.6280 Å b= 7.4670 Å c= 22.6070 Å α= 115.320° β= 80.560 ° γ= 95.490 °
I/Ic	0.54
Calc. density	3.954 g/cm <sup>3</sup>
Reference	Weber H. P., "Ferrosilite III, the high-temperature polymorph of FeSiO <sub>3</sub> ", <i>Acta Crystallographica, Section C</i> <b>39</b> , 1-3 (1983)
<b>E: Wollastonite-2M (10.5 %)*</b>	
Formula sum	Ca O3 Si
Entry number	98-901-1914
Figure-of-Merit (FoM)	0.829566 <sup>†</sup>
Total number of peaks	404
Peaks in range	404
Peaks matched	404
Intensity scale factor	0.38 <sup>†</sup>
Space group	P 1 21/a 1
Crystal system	monoclinic
Unit cell	a= 15.3800 Å b= 7.2850 Å c= 7.0840 Å β= 95.400 °
I/Ic	1.58
Calc. density	2.933 g/cm <sup>3</sup>
Reference	Mamedov K. S., Belov N. V., "The crystal structure of wollastonite", <i>Doklady Akademii Nauk SSSR</i> <b>107</b> , 463-466 (1956)
<b>F: Tridymite (7.6 %)*</b>	
Formula sum	O2 Si
Entry number	98-901-7299
Figure-of-Merit (FoM)	0.808309 <sup>†</sup>
Total number of peaks	287
Peaks in range	287
Peaks matched	286
Intensity scale factor	0.27 <sup>†</sup>
Space group	C 1 c 1
Crystal system	monoclinic

Unit cell: a = 18.418(3) Å b = 4.991(1) Å c = 7.636(2) Å β = 117.75(3)°  
 V<sub>0</sub>: 1.62  
 Calc. density: 2.270 g/cm<sup>3</sup>  
 Reference: Kato V. K., Nukui A., 'Die kristallstruktur des monoklinen tieftridymits', Acta Crystallographica, Section D 32 2430-2491 (1973)

<sup>(1)</sup> 2-theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

### Search-Match

**Settings**  
 Reference database used: COD-Inorg 2023.05.06  
 Automatic zero-point adaption: Yes  
 Downgrade phases with low scaling factors: Yes  
 Minimum figure-of-merit (FoM): 0.60  
 2-theta window for peak com.: 0.97 deg. (automatically determined)  
 Minimum rel. int. for peak com.: 0  
 Parameter/influence 2-theta: 0.50  
 Parameter/influence intensity: 0.50  
 Parameter multiplicity/phase(s): 0.50



Match! Copyright © 2003-2023 CRYSTAL IMPACT, Bonn, Germany



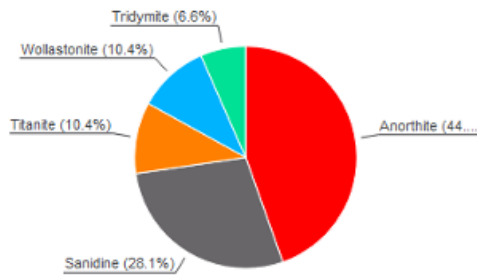
## Sample: TEST SAMPLE

### Sample Data

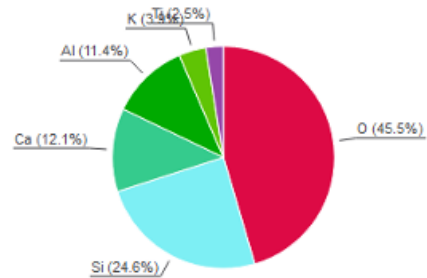
File name	BT_4 UNHAS.raw
File path	C:/Users/AGUNGP~1/AppData/Local/Temp/Rar\$DRa11372.1557/Hasil XRD
Data collected	Agu 18, 2022 04:05:55
Data range	9.920° - 89.920°
Original data range	10.000° - 90.000°
Number of points	4001
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	-0.08°
Radiation	X-rays
Wavelength	1.540598 Å

### Analysis Results

#### Phase composition (Weight %)



#### Elemental composition (Weight %)



#### Index Amount (%) Name

A	44.6	Anorthite
B	28.1	Sanidine
C	10.4	Titanite
D	10.4	Wollastonite
E	6.6	Tridymite
	1.6	Unidentified peak area

#### Formula sum

A	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
B	Al K O <sub>8</sub> Si <sub>3</sub>
C	Ca O <sub>5</sub> Si Ti
D	Ca O <sub>3</sub> Si
E	O <sub>2</sub> Si

#### Element Amount (weight %)

O	45.5% (*)
Si	24.6%
Ca	12.1%
Al	11.4%
K	3.9%
Ti	2.5%
*LE (sum)	45.5%

Amounts calculated by RIR (Reference Intensity Ratio) method

#### Details of identified phases

##### A: Anorthite (44.6 %) \*

Formula sum	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
Entry number	96-900-0362
Figure-of-Merit (FoM)	0.877793 <sup>†</sup>
Total number of peaks	499
Peaks in range	499
Peaks matched	494
Intensity scale factor	0.32 <sup>†</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 8.1940 Å b= 12.8970 Å c= 14.1900 Å α= 92.980° β= 115.820° γ= 91.150°
I/c	0.54
Calc. density	2.745 g/cm <sup>3</sup>
Reference	Foit F. F., Peacor D. R., "The anorthite crystal structure at 410 and 830 CT = 410 C", American Mineralogist 58,

665-675 (1973)

**B: Sanidine (28.1 %)<sup>†</sup>**

Formula sum	Al K O8 Si3
Entry number	98-900-4247
Figure-of-Merit (FoM)	0.794380 <sup>†</sup>
Total number of peaks	292
Peaks in range	292
Peaks matched	292
Intensity scale factor	0.28 <sup>†</sup>
Space group	C 1 2/m 1
Crystal system	monoclinic
Unit cell	a= 8.6110 Å b= 13.0460 Å c= 7.1750 Å β= 116.010 °
I/Ic	0.73
Calc. density	2.552 g/cm <sup>3</sup>
Reference	Ferguson R. B., Ball N. A., Cerny P., "Structure refinement of an adularian end-member high sanidine from the Buck Claim Pegmatite, Bernic Lake, Manitoba Sample: IIIINote: variety adularia", <i>The Canadian Mineralogist</i> <b>29</b> , 543-552 (1991)

**C: Titanite (10.4 %)<sup>†</sup>**

Formula sum	Ca O5 Si Ti
Entry number	98-900-2452
Figure-of-Merit (FoM)	0.813410 <sup>†</sup>
Total number of peaks	500
Peaks in range	295
Peaks matched	290
Intensity scale factor	0.17 <sup>†</sup>
Space group	P 1 21/a 1
Crystal system	monoclinic
Unit cell	a= 6.9820 Å b= 8.6748 Å c= 6.4924 Å β= 113.498 °
I/Ic	1.21
Calc. density	3.611 g/cm <sup>3</sup>
Reference	Kunz M., Arlt T., Stolz J., "In situ powder diffraction study of titanite (CaTiOSiO <sub>4</sub> ) at high pressure and high temperature Sample", <i>American Mineralogist</i> <b>85</b> , 1465-1473 (2000)

**D: Wollastonite (10.4 %)<sup>†</sup>**

Formula sum	Ca O3 Si
Entry number	98-900-5779
Figure-of-Merit (FoM)	0.803938 <sup>†</sup>
Total number of peaks	487
Peaks in range	487
Peaks matched	487
Intensity scale factor	0.24 <sup>†</sup>
Space group	P 1 21/a 1
Crystal system	monoclinic
Unit cell	a= 15.4240 Å b= 7.3240 Å c= 7.0692 Å β= 95.371 °
I/Ic	1.72
Calc. density	2.911 g/cm <sup>3</sup>
Reference	Ohashi Y., "Polysynthetically-twinned structures of enstatite and wollastonite Sample: WO2M", <i>Physics and Chemistry of Minerals</i> <b>10</b> , 217-229 (1984)

**E: Tridymite (6.6 %)<sup>†</sup>**

Formula sum	O2 Si
Entry number	98-900-6969
Figure-of-Merit (FoM)	0.815287 <sup>†</sup>
Total number of peaks	499
Peaks in range	499
Peaks matched	497
Intensity scale factor	0.12 <sup>†</sup>
Space group	P 21 21 21
Crystal system	orthorhombic
Unit cell	a= 26.1753 Å b= 4.9844 Å c= 8.2006 Å
I/Ic	1.38
Calc. density	2.238 g/cm <sup>3</sup>
Reference	Graetsch H., "X-ray powder diffraction study on the modulated high temperature forms of SiO <sub>2</sub> tridymite between 110 and 220 °C Sample: superstructure, T = 115 °C", <i>Physics and Chemistry of Minerals</i> <b>28</b> , 313-321 (2001)

<sup>†</sup>) 2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

## Integrated Profile Areas

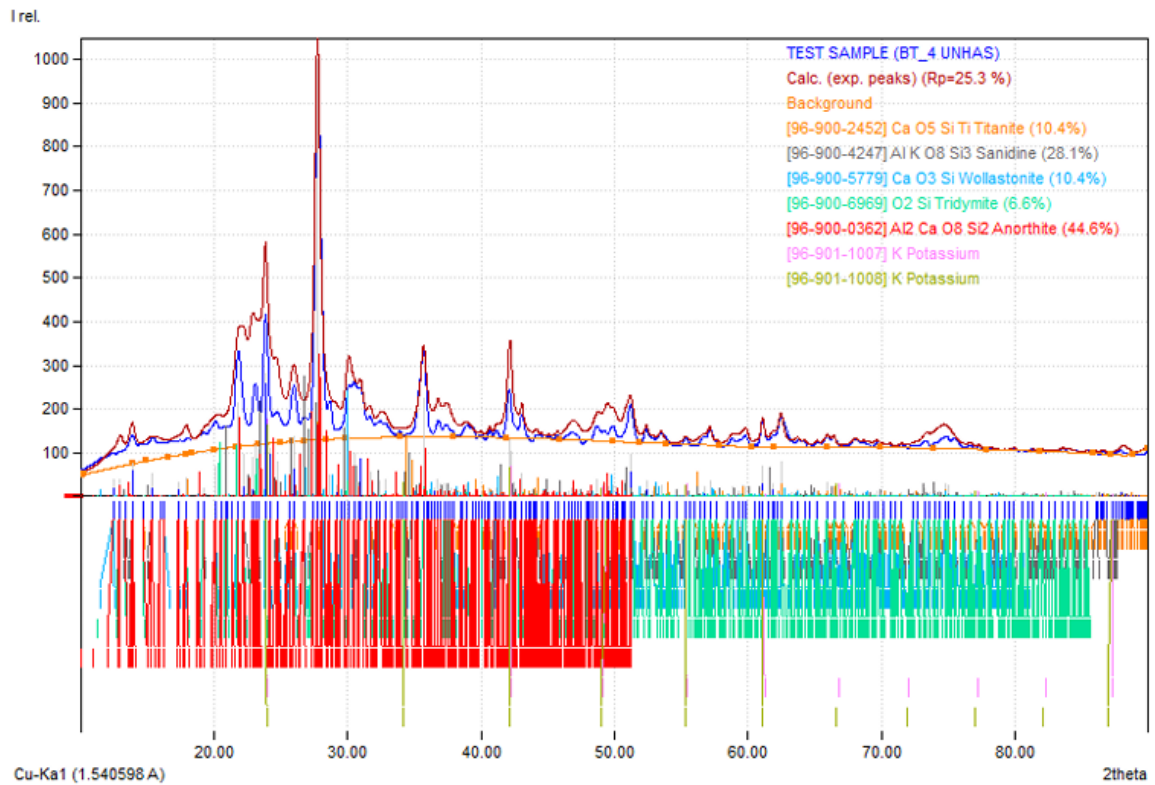
Based on calculated profile

Profile area	Counts	Amount
Overall diffraction profile	887049	100.00%
Background radiation	694387	78.28%
Diffraction peaks	192663	21.72%
Peak area belonging to selected phases	178324	20.10%
Peak area of phase A (Titanite)	20702	2.33%
Peak area of phase B (Sanidine)	51165	5.77%
Peak area of phase C (Wollastonite)	18958	2.14%
Peak area of phase D (Tridymite)	15913	1.79%
Peak area of phase E (Anorthite)	71566	8.07%
Unidentified peak area	14338	1.62%

## Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	6487	100.00%
Peak intensity belonging to selected phases	5667	87.36%
Unidentified peak intensity	820	12.64%

## Diffraction Pattern Graphics



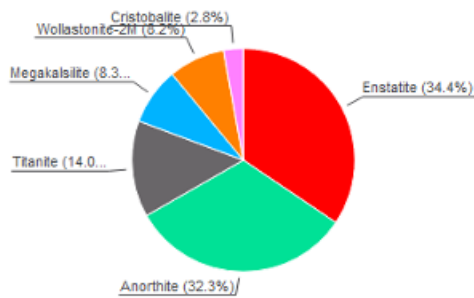
**Sample: TEST SAMPLE**

**Sample Data**

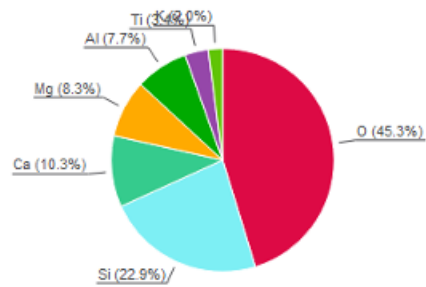
File name BT\_5 UNHAS.raw  
 File path C:/Users/AGUNGP-1/AppData/Local/Temp/Rar\$DRa11372.15346/Hasil XRD  
 Data collected Agu 18, 2022 03:19:38  
 Data range 10.000° - 90.000°  
 Original data range 10.000° - 90.000°  
 Number of points 4001  
 Step size 0.020  
 Rietveld refinement converged No  
 Alpha2 subtracted No  
 Background subtr. No  
 Data smoothed Yes  
 Radiation X-rays  
 Wavelength 1.540598 Å

**Analysis Results**

**Phase composition (Weight %)**



**Elemental composition (Weight %)**



Index	Amount (%)	Name	Formula sum	Element	Amount (weight %)
A	34.4	Enstatite	Mg O3 Si	O	45.3% (*)
B	32.3	Anorthite	Al2 Ca O8 Si2	Si	22.9%
C	14.0	Titanite	Ca O5 Si Ti	Ca	10.3%
D	8.3	Megakalsilite	Al K O4 Si	Mg	8.3%
E	8.2	Wollastonite-2M	Ca O3 Si	Al	7.7%
F	2.8	Cristobalite	O2 Si	Ti	3.4%
	1.5	Unidentified peak area		K	2.0%
				*LE (sum)	45.3%

Amounts calculated by RIR (Reference Intensity Ratio) method

**Details of identified phases**

**A: Enstatite (34.4 %)**  
 Formula sum Mg O3 Si  
 Entry number 96-900-6341  
 Figure-of-Merit (FoM) 0.843999<sup>\*</sup>  
 Total number of peaks 499  
 Peaks in range 362  
 Peaks matched 355  
 Intensity scale factor 0.53<sup>\*</sup>  
 Space group P b c a  
 Crystal system orthorhombic  
 Unit cell a= 18.4580 Å b= 8.9600 Å c= 5.2700 Å  
 I/Ic 0.69  
 Calc. density 3.061 g/cm<sup>3</sup>  
 Reference Yang H., Ghose S., "High temperature single crystal X-ray diffraction studies of the ortho-proto phase transition"

in enstatite, Mg<sub>2</sub>Si<sub>2</sub>O<sub>6</sub> at 1360 K Sample: T = 1380 K", *Physics and Chemistry of Minerals* **22**, 300-310 (1995)

**B: Anorthite (32.3 %)**\*

Formula sum Al<sub>2</sub> Ca O<sub>8</sub> Si<sub>2</sub>  
 Entry number 96-900-1260  
 Figure-of-Merit (FoM) 0.841315<sup>†</sup>  
 Total number of peaks 497  
 Peaks in range 497  
 Peaks matched 494  
 Intensity scale factor 0.39<sup>†</sup>  
 Space group P -1  
 Crystal system triclinic (anorthic)  
 Unit cell a= 8.1796 Å b= 12.8747 Å c= 14.1720 Å α= 93.134° β= 115.885° γ= 91.236°  
 I/Ic 0.54  
 Calc. density 2.780 g/cm<sup>3</sup>  
 Reference Angel R. J., Carpenter M. A., Finger L. W., "Structural variation associated with compositional variation and order-disorder behavior in anorthite-rich feldspars sample from Monte Somma", *American Mineralogist* **75**, 150-162 (1990)

**C: Titanite (14.0 %)**\*

Formula sum Ca O<sub>5</sub> Si Ti  
 Entry number 96-900-2480  
 Figure-of-Merit (FoM) 0.822365<sup>†</sup>  
 Total number of peaks 500  
 Peaks in range 299  
 Peaks matched 292  
 Intensity scale factor 0.41<sup>†</sup>  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 7.0014 Å b= 8.6869 Å c= 6.5081 Å β= 113.533°  
 I/Ic 1.33  
 Calc. density 3.588 g/cm<sup>3</sup>  
 Reference Kunz M., Arlt T., Stolz J., "In situ powder diffraction study of titanite (CaTiOSiO<sub>4</sub>) at high pressure and high temperature Sample", *American Mineralogist* **85**, 1465-1473 (2000)

**D: Megakalsilite (8.3 %)**\*

Formula sum Al K O<sub>4</sub> Si  
 Entry number 96-900-4686  
 Figure-of-Merit (FoM) 0.823587<sup>†</sup>  
 Total number of peaks 290  
 Peaks in range 290  
 Peaks matched 288  
 Intensity scale factor 0.38<sup>†</sup>  
 Space group P 63  
 Crystal system hexagonal  
 Unit cell a= 18.1111 Å c= 8.4619 Å  
 I/Ic 2.07  
 Calc. density 2.622 g/cm<sup>3</sup>  
 Reference Khomyakov A. P., Nechelyustov G. N., Sokolova E. V., Bonaccorsi E., Merlino S., Pasero M., "Megakalsilite, a new polymorph of KAlSiO<sub>4</sub> from the Khibina alkaline massif, Kola Peninsula, Russia: mineral description and crystal structure", *The Canadian Mineralogist* **40**, 961-970 (2002)

**E: Wollastonite-2M (8.2 %)**

Formula sum Ca O<sub>3</sub> Si  
 Entry number 96-900-8152  
 Figure-of-Merit (FoM) 0.825513  
 Total number of peaks 498  
 Peaks in range 498  
 Peaks matched 498  
 Intensity scale factor 0.32  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 15.4260 Å b= 7.3200 Å c= 7.0660 Å β= 95.404°  
 I/Ic 1.75  
 Calc. density 2.914 g/cm<sup>3</sup>  
 Reference Trojer F. J., "The crystal structure of parawollastonite", *Zeitschrift für Kristallographie* **127**, 291-308 (1968)

**F: Cristobalite (2.8 %)**\*

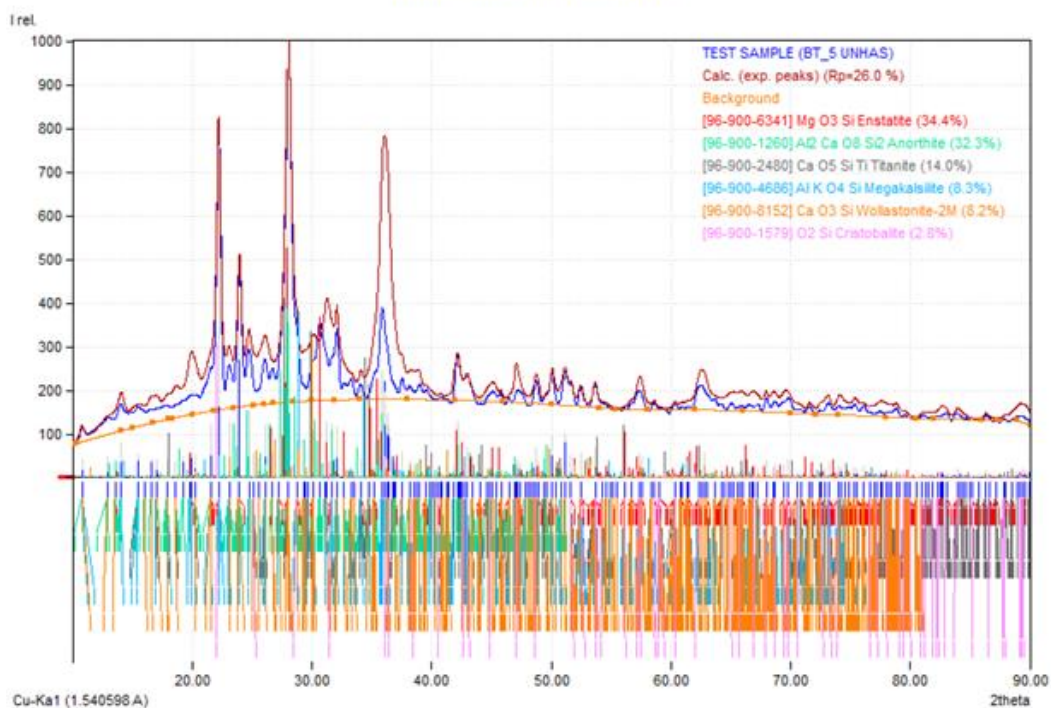
Formula sum O<sub>2</sub> Si  
 Entry number 96-900-1579  
 Figure-of-Merit (FoM) 0.725240<sup>†</sup>  
 Total number of peaks 134  
 Peaks in range 57  
 Peaks matched 56  
 Intensity scale factor 0.31<sup>†</sup>  
 Space group P 41 21 2  
 Crystal system tetragonal  
 Unit cell a= 4.9717 Å c= 6.9223 Å

Peak area of phase E (Wollastonite-2M)	19104	2.11%
Peak area of phase F (Cristobalite)	11046	1.22%
Unidentified peak area	13682	1.51%

### Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	8393	100.00%
Peak intensity belonging to selected phases	5135	80.32%
Unidentified peak intensity	1258	19.68%

### Diffraction Pattern Graphics



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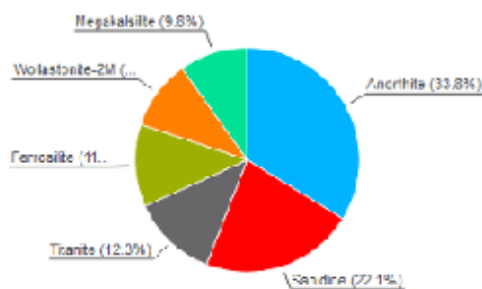
# Match! Phase Analysis Report

Sample: TFST SAMPI F

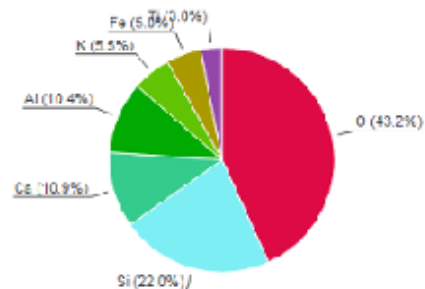
**Sample Data**  
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 File path: C:\Users\ACUNGP-1\AppData\Local\Temp\Ra\$DRa11372-0712\1\as1.XRD  
 Data collected: Agu 22, 2022 06:14:20  
 Data range: 10.000° - 90.000°  
 Original data range: 10.000° - 90.000°  
 Number of points: 4001  
 Step size: 0.020  
 Rietveld refinement converged: No  
 Alpha2 subramer: No  
 Background sum: No  
 Data smoothed: Yes  
 Radiation: X-rays  
 Wavelength: 1.540608 Å

## Analysis Results

**Phase composition (Weight %)**



**Elemental composition (Weight %)**



Index	Amount (%)	Name	Formula sum
A	33.0	Anorthite	Al <sub>2</sub> CaO <sub>8</sub> Si <sub>2</sub>
B	22.1	Sandine	Al <sub>2</sub> KO <sub>8</sub> Si <sub>3</sub>
C	12.3	Titanite	CaO <sub>5</sub> Si <sub>2</sub> Ti
D	11.9	Ferrosilite	FeO <sub>3</sub> Si
F	10.0	Wolastonite-2M	CaO <sub>3</sub> Si
F	9.8	Magakalsite	Al <sub>2</sub> KO <sub>4</sub> Si
	0.9	Unidentified peak area	

Element	Amount (weight %)
O	43.26(%)
Si	22.0%
Ca	10.9%
Al	10.4%
K	5.5%
Fe	5.0%
Ti	3.0%
%Ls (sum)	43.2%

Amounts calculated by RIR (Reference intensity Ratio) method

### Details of identified phases

**A: Anorthite (33.8 %)**  
 Formula sum: Al<sub>2</sub>CaO<sub>8</sub>Si<sub>2</sub>  
 Entry number: 08 000 1260  
 Figure-of-Merit (FOM): 0.829675  
 Total number of peaks: 400  
 Peaks in range: 400  
 Peaks matched: 106  
 Intensity scale factor: 0.43  
 Space group: P -1  
 Crystal system: triclinic (anorthite)  
 Unit cell: a= 8.1750 Å b= 12.8730 Å c= 14.1700 Å α= 93.110° β= 115.800° γ= 91.280°  
 V/c: 0.53  
 Calc. density: 2.783 g/cm<sup>3</sup>  
 Reference: Angel R. J., Carpenter M. A., Finger L. W., "Structural variation associated with compositional variation"

**B: Sanidine (22.1 %)\***

Formula sum Al K O8 Si3  
 Entry number 96-900-4245  
 Figure-of-Merit (FoM) 0.848291<sup>†</sup>  
 Total number of peaks 292  
 Peaks in range 292  
 Peaks matched 292  
 Intensity scale factor 0.39<sup>†</sup>  
 Space group C 1 2/m 1  
 Crystal system monoclinic  
 Unit cell a= 8.6030 Å b= 13.0360 Å c= 7.1740 Å β= 116.030 °  
 I/lc 0.73  
 Calc. density 2.557 g/cm<sup>3</sup>  
 Reference Ferguson R. B., Ball N. A., Cerny P., "Structure refinement of an adularian end-member high sanidine from the Buck Claim Pegmatite, Berric Lake, Manitoba Sample: INote: variety adularia". The Canadian Mineralogist **29**, 543-552 (1991)

**C: Titanite (12.3 %)\***

Formula sum Ca O5 Si Ti  
 Entry number 96-900-2479  
 Figure-of-Merit (FoM) 0.821116<sup>†</sup>  
 Total number of peaks 500  
 Peaks in range 295  
 Peaks matched 292  
 Intensity scale factor 0.39<sup>†</sup>  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 6.9984 Å b= 8.6846 Å c= 6.5063 Å β= 113.521 °  
 I/lc 1.31  
 Calc. density 3.591 g/cm<sup>3</sup>  
 Reference Kunz M., Arlt T., Stolz J., "In situ powder diffraction study of titanite (CaTiO5SiO4) at high pressure and high temperature Sample", American Mineralogist **85**, 1465-1473 (2000)

**D: Ferrosilite (11.9 %)\***

Formula sum Fe O3 Si  
 Entry number 96-900-6426  
 Figure-of-Merit (FoM) 0.799528<sup>†</sup>  
 Total number of peaks 490  
 Peaks in range 352  
 Peaks matched 341  
 Intensity scale factor 0.21<sup>†</sup>  
 Space group P b c a  
 Crystal system orthorhombic  
 Unit cell a= 18.3410 Å b= 8.9660 Å c= 5.1925 Å  
 I/lc 0.74  
 Calc. density 4.105 g/cm<sup>3</sup>  
 Reference Hugh-Jones D A, Chopelas A., Angel R. J., "Tetrahedral compression in (Mg,Fe)SiO3 orthopyroxenes Sample: P = 2.84 GPa", Physics and Chemistry of Minerals **24**, 301-310 (1997)

**E: Wollastonite-2M (10.0 %)\***

Formula sum Ca O3 Si  
 Entry number 96-901-1914  
 Figure-of-Merit (FoM) 0.835177<sup>†</sup>  
 Total number of peaks 404  
 Peaks in range 404  
 Peaks matched 404  
 Intensity scale factor 0.38<sup>†</sup>  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 15.3600 Å b= 7.2850 Å c= 7.0840 Å β= 95.400 °  
 I/lc 1.58  
 Calc. density 2.933 g/cm<sup>3</sup>  
 Reference Mamedov K. S., Belov N. V., "The crystal structure of wollastonite", Doklady Akademii Nauk SSSR **107**, 463-466 (1956)



**F: Megakalsilite (9.8 %)**  
 Formula sum Al K O4 Si  
 Entry number 96-900-4686  
 Figure-of-Merit (FoM) 0.856462  
 Total number of peaks 290  
 Peaks in range 290  
 Peaks matched 288  
 Intensity scale factor 0.49  
 Space group P 63

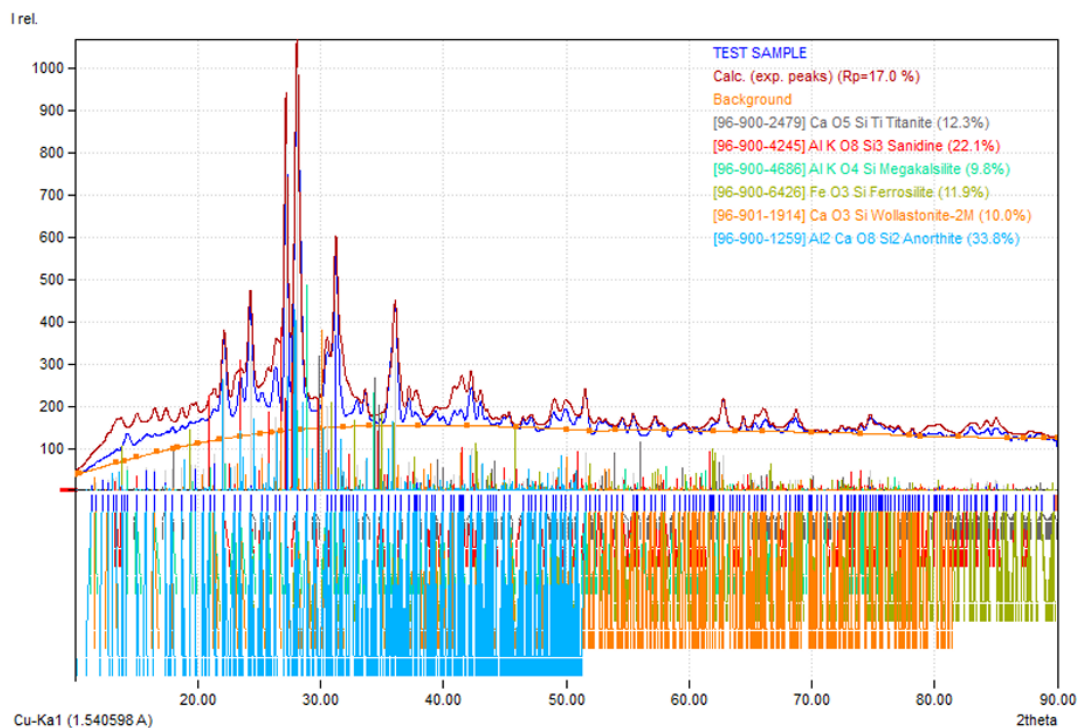
Crystal system hexagonal  
 Unit cell a= 18.1111 Å c= 8.4819 Å  
 I/c 2.07  
 Calc. density 2.622 g/cm<sup>3</sup>  
 Reference Khomyakov A. P., Nechelyustov G. N., Sokolova E. V., Bonaccorsi E., Merlino S., Pasero M., "Megakalsilite, a new polymorph of KAlSiO4 from the Khibina alkaline massif, Kola Peninsula, Russia: mineral description and crystal structure", The Canadian Mineralogist **40**, 961-970 (2002)

*(\*) 2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.*

### Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	5335	100.00%
Peak intensity belonging to selected phases	4847	90.86%
Unidentified peak intensity	488	9.14%

### Diffraction Pattern Graphics



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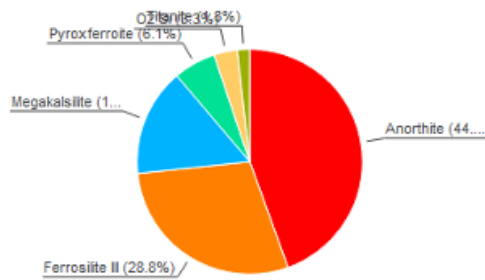
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### Sample Data

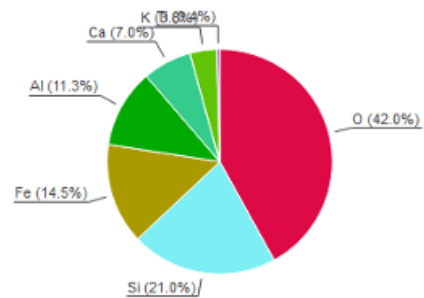
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Original data range	10.000° - 90.000°
Number of points	4001
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
Radiation	X-rays
Wavelength	1.540598 Å

## Analysis Results

**Phase composition (Weight %)**



**Elemental composition (Weight %)**



Index	Amount (%)	Name	Formula sum	Element	Amount (weight %)
A	44.5	Anorthite	Al2 Ca O8 Si2	O	42.0% (*)
B	28.8	Ferrosilite III	Fe O3 Si	Si	21.0%
C	15.5	Megakalsilite	Al K O4 Si	Fe	14.5%
D	6.1	Pyroxferroite	Ca0.94 Fe6.06 O21 Si7	Al	11.3%
E	3.3		O2 Si	Ca	7.0%
F	1.8	Titanite	Ca O5 Si Ti	K	3.8%
	6.5	Unidentified peak area		Ti	0.4%
				*LE (sum)	42.0%

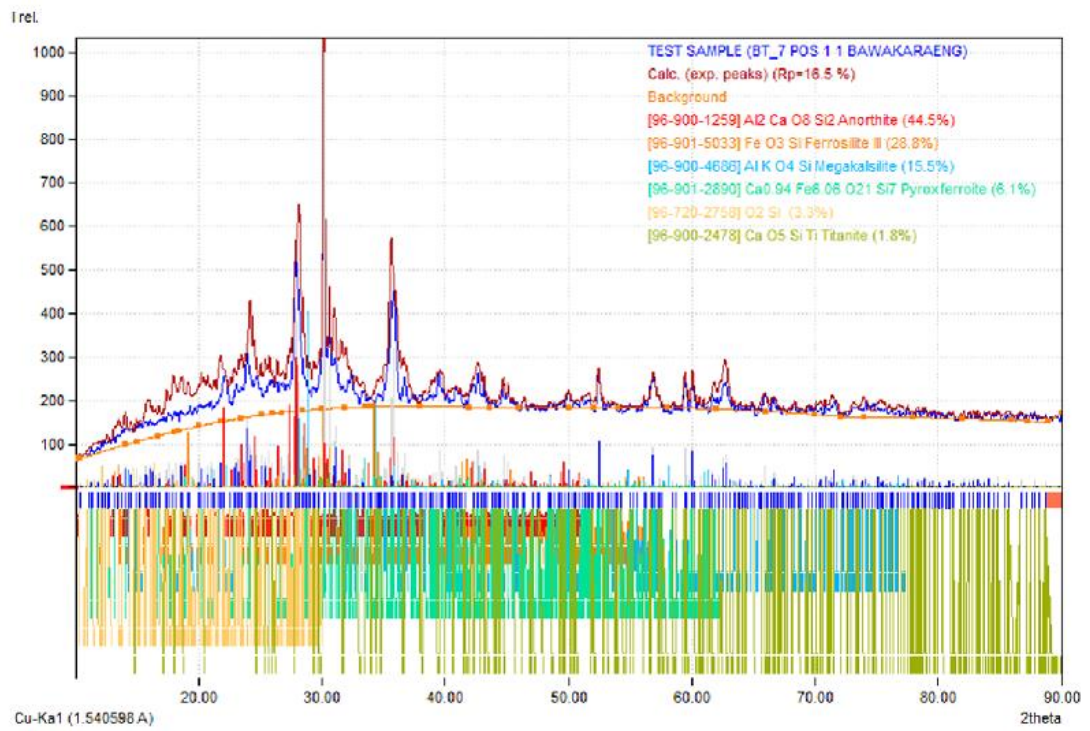
Amounts calculated by RIR (Reference Intensity Ratio) method

### Details of identified phases

#### A: Anorthite (44.5 %)

Formula sum	Al2 Ca O8 Si2
Entry number	96-900-1259
Figure-of-Merit (FoM)	0.894920
Total number of peaks	499
Peaks in range	499
Peaks matched	498
Intensity scale factor	0.30
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 8.1750 Å b= 12.8730 Å c= 14.1700 Å α= 93.110° β= 115.890° γ= 91.280°
I/c	0.53
Calc. density	2.763 g/cm <sup>3</sup>

Reference	Angel R. J., Carpenter M. A., Finger L. W., "Structural variation associated with compositional variation and order-disorder behavior in anorthite-rich feldspars sample from Val Pasmada", <i>American Mineralogist</i> <b>75</b> , 150-162 (1990)
<b>B: Ferrosilite III (28.8 %)</b>	
Formula sum	Fe O3 Si
Entry number	96-901-5033
Figure-of-Merit (FoM)	0.857694
Total number of peaks	499
Peaks in range	499
Peaks matched	497
Intensity scale factor	0.20
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 6.6280 Å b= 7.4670 Å c= 22.6070 Å α= 115.320° β= 80.560 ° γ= 95.490 °
I/Ic	0.54
Calc. density	3.954 g/cm <sup>3</sup>
Reference	Weber H. P., "Ferrosilite III, the high-temperature polymorph of FeSiO <sub>3</sub> ", <i>Acta Crystallographica, Section C</i> <b>39</b> , 1-3 (1983)
<b>C: Megakalsilite (15.5 %)</b>	
Formula sum	Al K O4 Si
Entry number	96-900-4686
Figure-of-Merit (FoM)	0.857552
Total number of peaks	290
Peaks in range	290
Peaks matched	288
Intensity scale factor	0.40
Space group	P 63
Crystal system	hexagonal
Unit cell	a= 18.1111 Å c= 8.4619 Å
I/Ic	2.07
Calc. density	2.622 g/cm <sup>3</sup>
Reference	Khomyakov A. P., Nechelyustov G. N., Sokolova E. V., Bonaccorsi E., Merlino S., Pasero M., "Megakalsilite, a new polymorph of KAlSiO <sub>4</sub> from the Khibina alkaline massif, Kola Peninsula, Russia: mineral description and crystal structure", <i>The Canadian Mineralogist</i> <b>40</b> , 961-970 (2002)
<b>D: Pyroxferroite (6.1 %)</b>	
Formula sum	Ca0.94 Fe6.06 O21 Si7
Entry number	96-901-2890
Figure-of-Merit (FoM)	0.860753
Total number of peaks	496
Peaks in range	496
Peaks matched	495
Intensity scale factor	0.07
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 6.6213 Å b= 7.5506 Å c= 17.3806 Å α= 114.267° β= 82.684 ° γ= 94.576 °
I/Ic	0.89
Calc. density	3.843 g/cm <sup>3</sup>
Reference	Burnham C. W., "The crystal structure of pyroxferroite from Mare Tranquillitatis", <i>Proceedings of the Second Lunar Science Conference</i> <b>1</b> , 47-57 (1971)
<b>E: O2 Si (3.3 %)</b>	
Formula sum	O2 Si
Entry number	96-720-2758
Figure-of-Merit (FoM)	0.787747
Total number of peaks	183
Peaks in range	183
Peaks matched	172
Intensity scale factor	0.05
Space group	P 1
Crystal system	triclinic (anorthic)
Unit cell	a= 14.4859 Å b= 10.0372 Å c= 43.0025 Å α= 90.000° β= 90.000 ° γ= 90.000 °
I/Ic	1.27
Calc. density	1.531 g/cm <sup>3</sup>
Reference	Bromley Stefan T., "A computational study into the viability of new molecular materials/polymorphs based on fully-coordinated inorganic nanoclusters", <i>CrystEngComm</i> <b>9(6)</b> , 463 (2007)
<b>F: Titanite (1.8 %)</b>	
Formula sum	Ca O5 Si Ti
Entry number	96-900-2478
Figure-of-Merit (FoM)	0.835359



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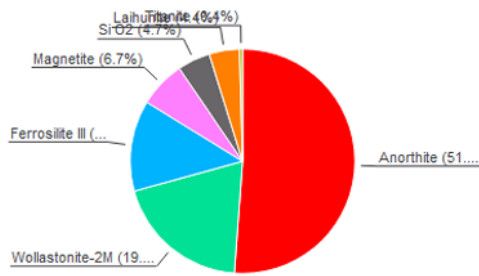
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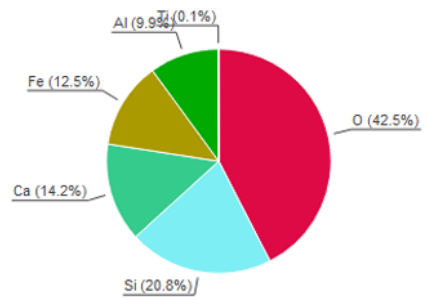
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 Number of points 4001  
 Step size 0.020  
 Rietveld refinement converged No  
 Alpha2 subtracted No  
 Background subtr. No  
 Data smoothed Yes  
 2theta correction 0.29°  
 Radiation X-rays  
 Wavelength 1.540598 Å

**Analysis Results**

**Phase composition (Weight %)**



**Elemental composition (Weight %)**



**Index Amount (%) Name**

A	51.2	Anorthite
B	19.5	Wollastonite-2M
C	13.1	Ferrosilite III
D	6.7	Magnetite
E	4.7	Si O2
F	4.4	Lahnunite
G	0.4	Titanite
	5.2	Unidentified peak area

**Formula sum**

Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
Ca O <sub>3</sub> Si
Fe O <sub>3</sub> Si
Fe <sub>3</sub> O <sub>4</sub>
O <sub>2</sub> Si
Fe <sub>4.74</sub> O <sub>12</sub> Si <sub>3</sub>
Ca O <sub>5</sub> Si Ti

**Element Amount (weight %)**

O	42.5% (*)
Si	20.8%
Ca	14.2%
Fe	12.5%
Al	9.9%
Ti	0.1%
*LE (sum)	42.5%

Amounts calculated by RIR (Reference Intensity Ratio) method

<b>A: Anorthite (51.2 %)*</b>	
Formula sum	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
Entry number	96-900-0363
Figure-of-Merit (FoM)	0.909709*
Total number of peaks	500
Peaks in range	500
Peaks matched	495
Intensity scale factor	0.39*
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 8.2230 Å b= 12.9150 Å c= 14.2040 Å α= 92.750° β= 115.800 ° γ= 91.020 °
I/Ic	0.51
<hr/>	
Calc. density	2.727 g/cm <sup>3</sup>
Reference	Foit F. F., Peacor D. R., "The anorthite crystal structure at 410 and 830 CT = 830 C", American Mineralogist <b>58</b> , 665-675 (1973)
<b>B: Wollastonite-2M (19.5 %)*</b>	
Formula sum	Ca O <sub>3</sub> Si
Entry number	96-901-1914
Figure-of-Merit (FoM)	0.864853*
Total number of peaks	404
Peaks in range	404
Peaks matched	404
Intensity scale factor	0.46*
Space group	P 1 21/a 1
Crystal system	monoclinic
Unit cell	a= 15.3600 Å b= 7.2850 Å c= 7.0840 Å β= 95.400 °
I/Ic	1.58
Calc. density	2.933 g/cm <sup>3</sup>
Reference	Mamedov K. S., Belov N. V., "The crystal structure of wollastonite", Doklady Akademii Nauk SSSR <b>107</b> , 463-466 (1956)
<b>C: Ferrosilite III (13.1 %)</b>	
Formula sum	Fe O <sub>3</sub> Si
Entry number	96-901-5033
Figure-of-Merit (FoM)	0.846203
Total number of peaks	499
Peaks in range	499
Peaks matched	497
Intensity scale factor	0.10
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 6.6280 Å b= 7.4670 Å c= 22.6070 Å α= 115.320° β= 80.560 ° γ= 95.490 °
I/Ic	0.54
Calc. density	3.954 g/cm <sup>3</sup>
Reference	Weber H. P., "Ferrosilite III, the high-temperature polymorph of FeSiO <sub>3</sub> ", Acta Crystallographica, Section C <b>39</b> , 1-3 (1983)
<b>D: Magnetite (6.7 %)*</b>	
Formula sum	Fe <sub>3</sub> O <sub>4</sub>
Entry number	96-900-5814
Figure-of-Merit (FoM)	0.734912*
Total number of peaks	36
Peaks in range	17
Peaks matched	17
Intensity scale factor	0.58*
Space group	F d -3 m
Crystal system	cubic
Unit cell	a= 8.3578 Å
I/Ic	5.82
Calc. density	5.268 g/cm <sup>3</sup>
Reference	Fingerl W., Hazen R. M., Hofmeister A. M., "High-pressure crystal chemistry of spinel (MgAl <sub>2</sub> O <sub>4</sub> ) and

**E: Si O2 (4.7 %)\***

Formula sum	O2 Si
Entry number	96-412-4066
Figure-of-Merit (FoM)	0.847387
Total number of peaks	491
Peaks in range	470
Peaks matched	469
Intensity scale factor	0.11*
Space group	P b c a
Crystal system	orthorhombic
Unit cell	a= 8.7724 Å b= 8.7833 Å c= 16.1865 Å
I/c	1.51
Calc. density	2.559 g/cm <sup>3</sup>
Reference	Foster M.D., Friedrichs O.D., Bell R.G., Paz F.A.A., Klinowski J., "Chemical evaluation of hypothetical uninodal zeolites", Journal of the American Chemical Society <b>126</b> , 9769-9775 (2004)

**F: Laihunite (4.4 %)**

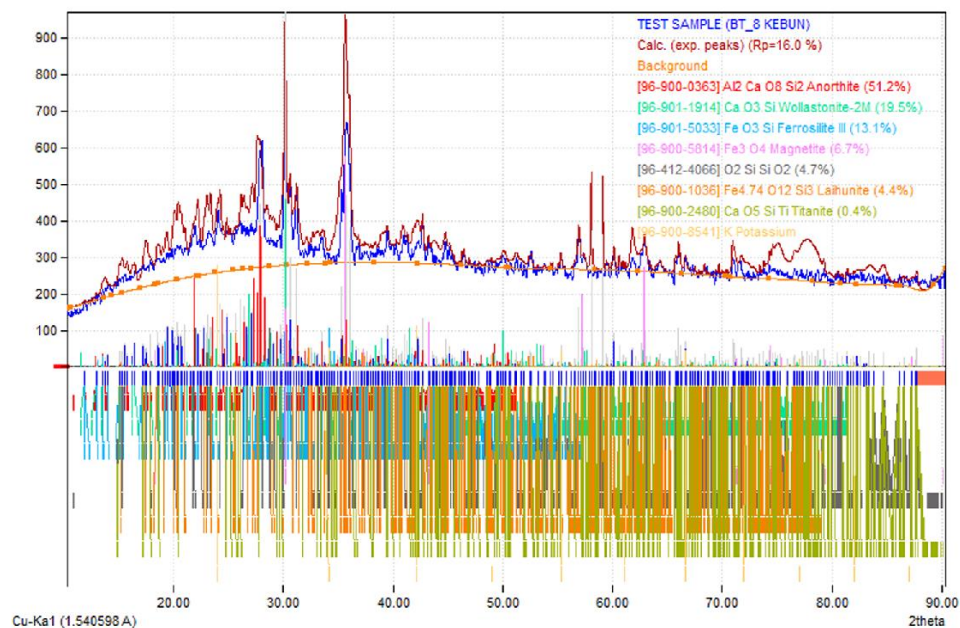
Formula sum	Fe4.74 O12 Si3
Entry number	96-900-1036
Figure-of-Merit (FoM)	0.848808
Total number of peaks	497
Peaks in range	497
Peaks matched	495
Intensity scale factor	0.09
Space group	P 21/b 1 1
Crystal system	monoclinic

Unit cell	a= 4.8050 Å b= 10.1890 Å c= 17.4030 Å α= 91.000°
I/c	1.40
Calc. density	4.218 g/cm <sup>3</sup>
Reference	Shen B., Tamada O., Kitamura M., Morimoto N., "Superstructure of laihunite-3M (L <sub>40</sub> Fe <sub>80</sub> SiO <sub>4</sub> )Sample: SuperstructureFe1B-y coordinate changed by Tamada (Aug, 2001)", American Mineralogist <b>71</b> , 1455-1460 (1986)

**G: Titanite (0.4 %)\***

Formula sum	Ca O5 Si Ti
Entry number	96-900-2480
Figure-of-Merit (FoM)	0.829837*
Total number of peaks	500
Peaks in range	280
Peaks matched	280
Intensity scale factor	0.01*
Space group	P 1 21/a 1
Crystal system	monoclinic
Unit cell	a= 7.0014 Å b= 8.6869 Å c= 6.5081 Å β= 113.533 °
I/c	1.33
Calc. density	3.588 g/cm <sup>3</sup>
Reference	Kunz M., Arit T., Stolz J., "In situ powder diffraction study of titanite (CaTiOSiO <sub>4</sub> ) at high pressure and high temperatureSample", American Mineralogist <b>85</b> , 1465-1473 (2000)

(\*) 2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.



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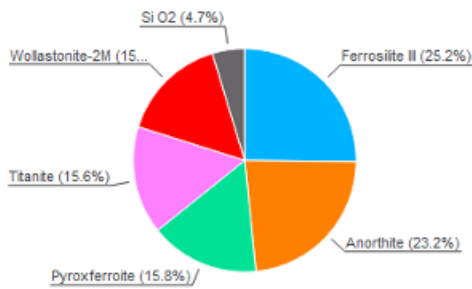
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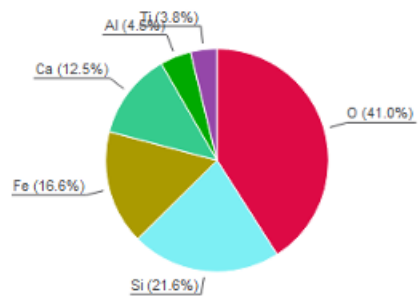
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 Step size 0.020  
 Rietveld refinement converged No  
 Alpha2 subtracted No  
 Background subtr. No  
 Data smoothed Yes  
 2theta correction -0.27°  
 Radiation X-rays  
 Wavelength 1.540598 Å

Analysis Results

Phase composition (Weight %)



Elemental composition (Weight %)



Index	Amount (%)	Name	Formula sum
A	25.2	Ferrosiite III	Fe O3 Si
B	23.2	Anorthite	Al2 Ca O8 Si2
C	15.8	Pyroxferroite	Ca0.94 Fe8.08 O21 Si7
D	15.6	Titanite	Ca O5 Si Ti
E	15.5	Wollastonite-2M	Ca O3 Si
F	4.7	Si O2	O2 Si
	0.3	Unidentified peak area	

Element	Amount (weight %)
O	41.0% (*)
Si	21.6%
Fe	16.6%
Ca	12.5%
Al	4.5%
Ti	3.8%
%LE (sum)	41.0%

Amounts calculated by RIR (Reference Intensity Ratio) method

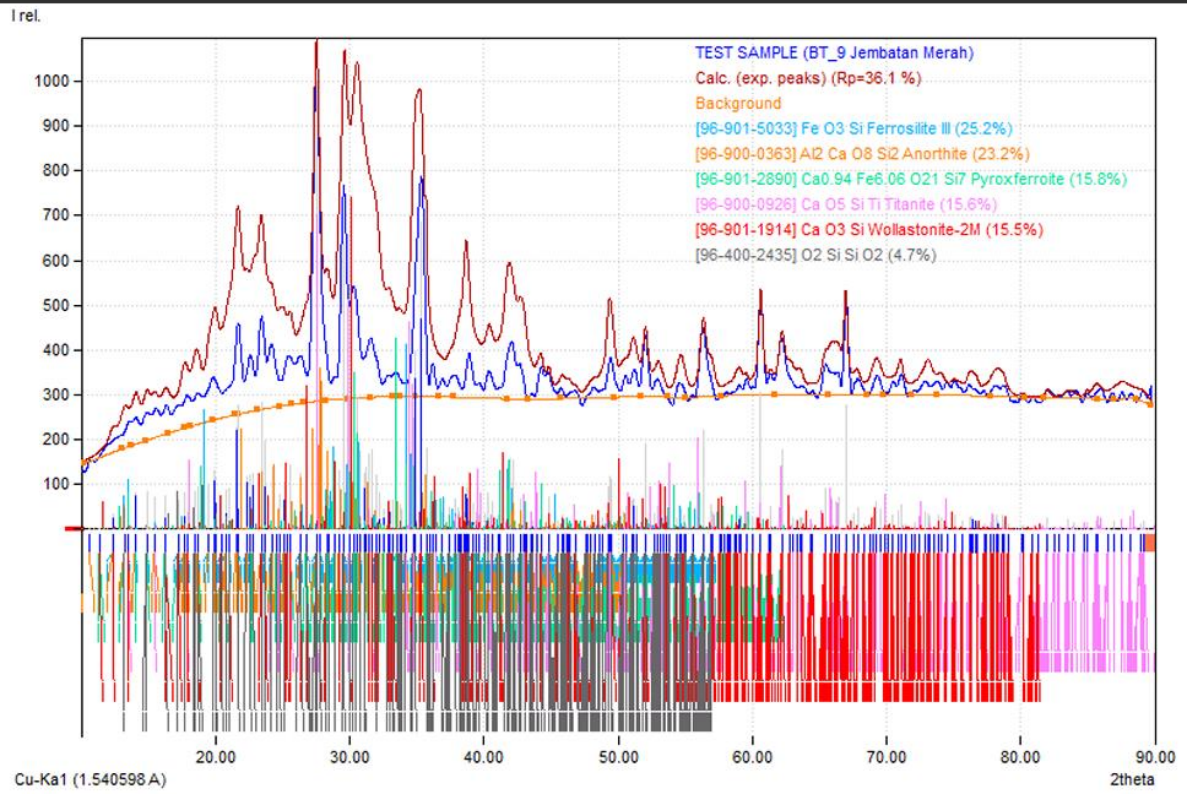
Details of identified phases

A: Ferrosiite III (25.2 %)\*

Formula sum Fe O3 Si  
 Entry number 96-901-5033  
 Figure-of-Merit (FoM) 0.846372<sup>2</sup>  
 Total number of peaks 499  
 Peaks in range 499  
 Peaks matched 497  
 Intensity scale factor 0.41<sup>1</sup>  
 Space group P -1  
 Crystal system triclinic (anorthic)  
 Unit cell a= 8.6280 Å b= 7.4670 Å c= 22.8070 Å α= 115.320° β= 80.560 ° γ= 95.490 °  
 I/Ic 0.54



Calc. density	3.954 g/cm <sup>3</sup>
Reference	Weber H. P., "Ferrosilite III, the high-temperature polymorph of FeSiO <sub>3</sub> ", Acta Crystallographica, Section C 39, 1-3 (1983)
<b>B: Anorthite (23.2 %)<sup>†</sup></b>	
Formula sum	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
Entry number	96-900-0363
Figure-of-Merit (FoM)	0.848268 <sup>†</sup>
Total number of peaks	500
Peaks in range	500
Peaks matched	497
Intensity scale factor	0.36 <sup>†</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 8.2230 Å b= 12.9150 Å c= 14.2040 Å α= 92.750° β= 115.800° γ= 91.020°
I/Ic	0.51
Calc. density	2.727 g/cm <sup>3</sup>
Reference	Foit F. F., Peacor D. R., "The anorthite crystal structure at 410 and 830 CT = 830 C", American Mineralogist 58, 665-675 (1973)
<b>C: Pyroxferroite (15.8 %)<sup>†</sup></b>	
Formula sum	Ca <sub>0.94</sub> Fe <sub>6.06</sub> O <sub>21</sub> Si <sub>7</sub>
Entry number	96-901-2890
Figure-of-Merit (FoM)	0.851702 <sup>†</sup>
Total number of peaks	496
Peaks in range	496
Peaks matched	495
Intensity scale factor	0.43 <sup>†</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 6.6213 Å b= 7.5506 Å c= 17.3806 Å α= 114.267° β= 82.684° γ= 94.576°
I/Ic	0.89
Calc. density	3.843 g/cm <sup>3</sup>
Reference	Burnham C. W., "The crystal structure of pyroxferroite from Mare Tranquillitatis", Proceedings of the Second Lunar Science Conference 1, 47-57 (1971)
<b>D: Titanite (15.6 %)<sup>†</sup></b>	
Formula sum	Ca O <sub>5</sub> Si Ti
Entry number	96-900-0926
Figure-of-Merit (FoM)	0.838971 <sup>†</sup>
Total number of peaks	500
Peaks in range	324
Peaks matched	319
Intensity scale factor	0.70 <sup>†</sup>
Space group	P 1 21 1
Crystal system	monoclinic
Unit cell	a= 7.0500 Å b= 8.6810 Å c= 6.5390 Å β= 113.900°
I/Ic	1.48
Calc. density	3.559 g/cm <sup>3</sup>
Reference	Hollabaugh C. L., Foit F. F., "The crystal structure of an Al-rich titanite from Grisons, Switzerland", American Mineralogist 69, 725-732 (1984)
<b>E: Wollastonite-2M (15.5 %)<sup>†</sup></b>	
Formula sum	Ca O <sub>3</sub> Si
Entry number	96-901-1914
Figure-of-Merit (FoM)	0.858844 <sup>†</sup>
Total number of peaks	404
Peaks in range	404
Peaks matched	404
Intensity scale factor	0.74 <sup>†</sup>
Space group	P 1 21/a 1
Crystal system	monoclinic
Unit cell	a= 15.3600 Å b= 7.2850 Å c= 7.0840 Å β= 95.400°
I/Ic	1.58
Calc. density	2.933 g/cm <sup>3</sup>
Reference	Mamedov K. S., Belov N. V., "The crystal structure of wollastonite", Doklady Akademii Nauk SSSR 107, 463-466 (1956)
<b>F: Si O<sub>2</sub> (4.7 %)<sup>†</sup></b>	
Formula sum	O <sub>2</sub> Si
Entry number	96-400-2435
Figure-of-Merit (FoM)	0.840034 <sup>†</sup>
Total number of peaks	486
Peaks in range	486



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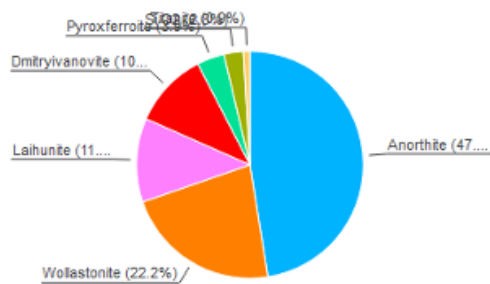
## Sample: TEST SAMPLE

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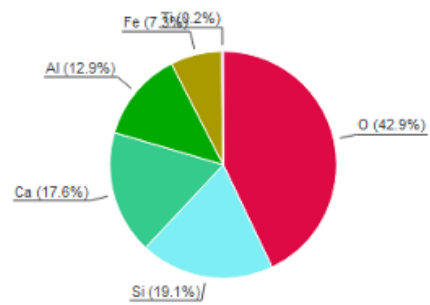
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Data collected	Agu 14, 2022 08:01:55
Data range	9.870° - 89.870°
Original data range	10.000° - 90.000°
Number of points	4001
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	Yes
2theta correction	-0.13°
Radiation	X-rays
Wavelength	1.540598 Å

## Analysis Results

**Phase composition (Weight %)**



**Elemental composition (Weight %)**



Index	Amount (%)	Name	Formula sum
A	47.5	Anorthite	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
B	22.2	Wollastonite	Ca O <sub>3</sub> Si
C	11.9	Laihunite	Fe <sub>4.74</sub> O <sub>12</sub> Si <sub>3</sub>
D	10.8	Dmitriyivanovite	Al <sub>2</sub> Ca O <sub>4</sub>
E	3.9	Pyroxferroite	Ca <sub>0.94</sub> Fe <sub>6.08</sub> O <sub>21</sub> Si <sub>7</sub>
F	2.8	Si O <sub>2</sub>	O <sub>2</sub> Si
G	0.9	Titanite	Ca O <sub>5</sub> Si Ti
	6.7	Unidentified peak area	

Element	Amount (weight %)
O	42.9% (*)
Si	19.1%
Ca	17.6%
Al	12.9%
Fe	7.3%
Ti	0.2%
*LE (sum)	42.9%

Amounts calculated by RIR (Reference Intensity Ratio) method

### Details of identified phases

**A: Anorthite (47.5 %)\***

Formula sum	Al <sub>2</sub> Ca O <sub>8</sub> Si <sub>2</sub>
Entry number	96-900-1280
Figure-of-Merit (FoM)	0.886934 <sup>2</sup>
Total number of peaks	497
Peaks in range	497
Peaks matched	494
Intensity scale factor	0.42 <sup>2</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a = 8.1796 Å b = 12.8747 Å c = 14.1720 Å α = 93.134° β = 115.885° γ = 91.236°

I/Ic	0.54
Calc. density	2.760 g/cm <sup>3</sup>
Reference	Angel R. J., Carpenter M. A., Finger L. W., "Structural variation associated with compositional variation and order-disorder behavior in anorthite-rich feldspars sample from Monte Somma", <i>American Mineralogist</i> <b>75</b> , 150-162 (1990)
<b>B: Wollastonite (22.2 %)</b> <sup>†</sup>	
Formula sum	Ca O3 Si
Entry number	96-900-5779
Figure-of-Merit (FoM)	0.867757 <sup>†</sup>
Total number of peaks	487
Peaks in range	487
Peaks matched	487
Intensity scale factor	0.63 <sup>†</sup>
Space group	P 1 21/a 1
Crystal system	monoclinic
Unit cell	a= 15.4240 Å b= 7.3240 Å c= 7.0692 Å β= 95.371 °
I/Ic	1.72
Calc. density	2.911 g/cm <sup>3</sup>
Reference	Ohashi Y., "Polysynthetically-twinned structures of enstatite and wollastonite Sample: WO2M", <i>Physics and Chemistry of Minerals</i> <b>10</b> , 217-229 (1984)
<b>C: Laihunite (11.9 %)</b> <sup>†</sup>	
Formula sum	Fe4.74 O12 Si3
Entry number	96-900-1036
Figure-of-Merit (FoM)	0.846087 <sup>†</sup>
Total number of peaks	497
Peaks in range	497
Peaks matched	496
Intensity scale factor	0.27 <sup>†</sup>
Space group	P 21/b 1 1
Crystal system	monoclinic
Unit cell	a= 4.8050 Å b= 10.1890 Å c= 17.4030 Å α= 91.000°
I/Ic	1.40
Calc. density	4.218 g/cm <sup>3</sup>
Reference	Shen B., Tamada O., Kitamura M., Morimoto N., "Superstructure of laihunite-3M (_40Fe.80Fe.80SiO4) Sample: Superstructure Fe1B-y coordinate changed by Tamada (Aug. 2001)", <i>American Mineralogist</i> <b>71</b> , 1455-1460 (1986)
<b>D: Dmitryivanovite (10.8 %)</b> <sup>†</sup>	
Formula sum	Al2 Ca O4
Entry number	96-901-3918
Figure-of-Merit (FoM)	0.871266 <sup>†</sup>
Total number of peaks	498
Peaks in range	498
Peaks matched	498
Intensity scale factor	0.15 <sup>†</sup>
Space group	P 1 21/c 1
Crystal system	monoclinic
Unit cell	a= 7.9719 Å b= 8.6284 Å c= 10.2628 Å β= 94.801 °
I/Ic	0.84
Calc. density	2.985 g/cm <sup>3</sup>
Reference	Lazic B., Kahlenberg V., Konzett J., "Structural studies on a stuffed framework high pressure polymorph of CaAl2O4", <i>Zeitschrift für Kristallographie</i> <b>222</b> , 890-895 (2007)
<b>E: Pyroxferroite (3.9 %)</b> <sup>†</sup>	
Formula sum	Ca0.94 Fe6.06 O21 Si7
Entry number	96-901-2890
Figure-of-Merit (FoM)	0.870906 <sup>†</sup>
Total number of peaks	496
Peaks in range	496
Peaks matched	495
Intensity scale factor	0.06 <sup>†</sup>
Space group	P -1
Crystal system	triclinic (anorthic)
Unit cell	a= 6.6213 Å b= 7.5506 Å c= 17.3806 Å α= 114.267° β= 82.684 ° γ= 94.576 °
I/Ic	0.89
Calc. density	3.843 g/cm <sup>3</sup>
Reference	Burnham C. W., "The crystal structure of pyroxferroite from Mare Tranquillitatis", <i>Proceedings of the Second Lunar Science Conference</i> <b>1</b> , 47-57 (1971)
<b>F: Si O2 (2.8 %)</b> <sup>†</sup>	
Formula sum	O2 Si
Entry number	96-412-4032

Figure-of-Merit (FoM) 0.846665<sup>†</sup>  
 Total number of peaks 212  
 Peaks in range 212

Peaks matched 211  
 Intensity scale factor 0.37<sup>†</sup>  
 Space group I 41/a m d  
 Crystal system tetragonal  
 Unit cell a= 10.0340 Å c= 20.6038 Å  
 I/lc 8.22  
 Calc. density 1.539 g/cm<sup>3</sup>  
 Reference Foster M.D., Friedrichs O.D., Bell R.G., Paz F.A.A., Klinowski J., "Chemical evaluation of hypothetical uninodal zeolites", Journal of the American Chemical Society **126**, 9769-9775 (2004)

**G: Titanite (0.9 %)**<sup>†</sup>  
 Formula sum Ca O5 Si Ti  
 Entry number 96-900-2439  
 Figure-of-Merit (FoM) 0.823440<sup>†</sup>  
 Total number of peaks 499  
 Peaks in range 293  
 Peaks matched 293  
 Intensity scale factor 0.02<sup>†</sup>  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 7.0442 Å b= 8.7132 Å c= 6.5476 Å β= 113.705 °  
 I/lc 1.47  
 Calc. density 3.539 g/cm<sup>3</sup>  
 Reference Kunz M., Arlt T., Stolz J., "In situ powder diffraction study of titanite (CaTiO5SiO4) at high pressure and high temperature", American Mineralogist **85**, 1465-1473 (2000)

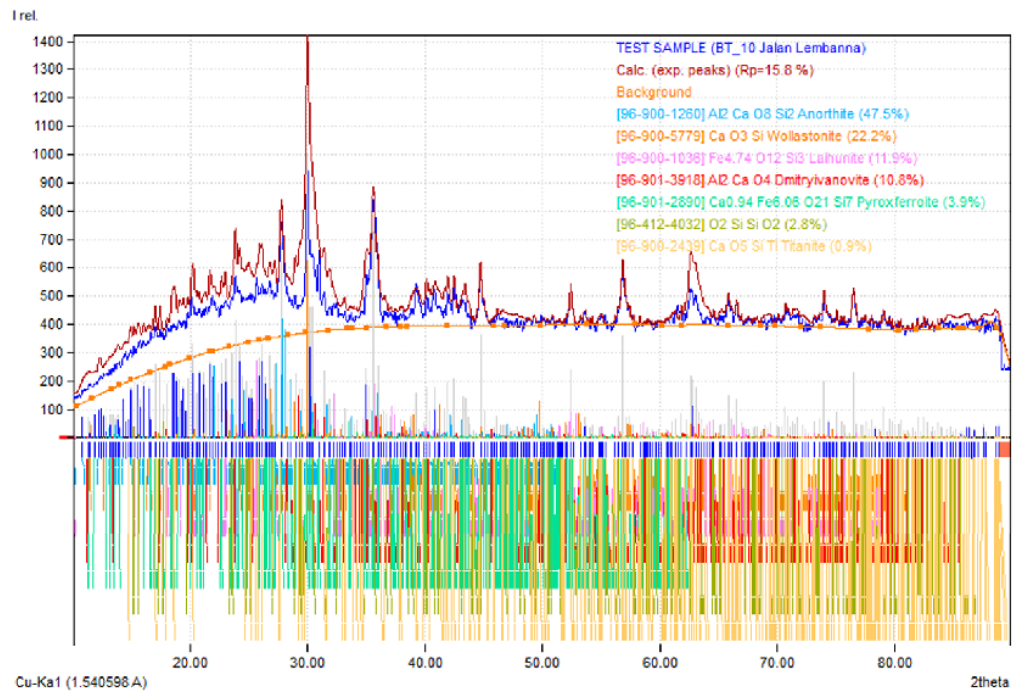
<sup>†</sup> 2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

Profile area	Counts	Amount
Overall diffraction profile	921597	100.00%
Background radiation	783119	84.97%
Diffraction peaks	138478	15.03%
Peak area belonging to selected phases	76392	8.29%
Peak area of phase A (Anorthite)	28891	3.13%
Peak area of phase B (Wollastonite)	18037	1.96%
Peak area of phase C (Laihunite)	12951	1.41%
Peak area of phase D (Dmitryivanovite)	9170	0.99%
Peak area of phase E (Pyroxferroite)	3530	0.38%
Peak area of phase F (Si O2)	2970	0.32%
Peak area of phase G (Titanite)	842	0.09%
Unidentified peak area	62086	6.74%

### Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	4481	100.00%
Peak intensity belonging to selected phases	3934	87.79%
Unidentified peak intensity	547	12.21%

### Diffraction Pattern Graphics



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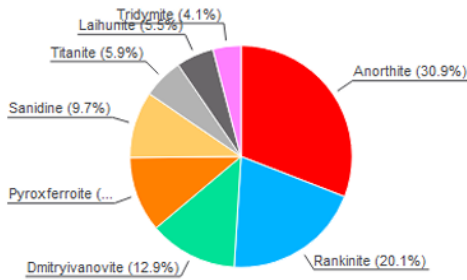
**Sample: TEST SAMPLE**

**Sample Data**

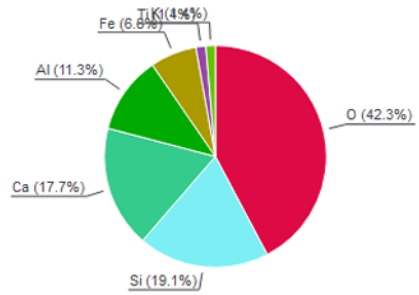
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 Data collected Agu 18, 2022 05:37:48  
 Data range 10.080° - 90.080°  
 Original data range 10.000° - 90.000°  
 Number of points 4001  
 Step size 0.020  
 Rietveld refinement converged No  
 Alpha2 subtracted No  
 Background subtr. No  
 Data smoothed Yes  
 2theta correction 0.08°  
 Radiation X-rays  
 Wavelength 1.540598 Å

**Analysis Results**

**Phase composition (Weight %)**



**Elemental composition (Weight %)**



Index	Amount (%)	Name	Formula sum	Element	Amount (weight %)
A	30.9	Anorthite	Al <sub>2</sub> CaO <sub>8</sub> Si <sub>2</sub>	O	42.3% (*)
B	20.1	Rankinite	Ca <sub>3</sub> O <sub>7</sub> Si <sub>2</sub>	Si	19.1%
C	12.9	Dmitryivanovite	Al <sub>2</sub> CaO <sub>4</sub>	Ca	17.7%
D	11.0	Pyroxferroite	Ca <sub>0.94</sub> Fe <sub>6.06</sub> O <sub>21</sub> Si <sub>7</sub>	Al	11.3%
E	9.7	Sanidine	AlK <sub>2</sub> O <sub>8</sub> Si <sub>3</sub>	Fe	6.8%
F	5.9	Titanite	CaO <sub>5</sub> SiTi	Ti	1.4%
G	5.5	Laihunite	Fe <sub>4.74</sub> O <sub>12</sub> Si <sub>3</sub>	K	1.4%
H	4.1	Tridymite	O <sub>2</sub> Si	*LE (sum)	42.3%
	2.7	Unidentified peak area			

Amounts calculated by RIR (Reference Intensity Ratio) method

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**Details of identified phases****A: Anorthite (30.9 %)\***

Formula sum Al<sub>2</sub> Ca O<sub>8</sub> Si<sub>2</sub>  
Entry number 96-900-1260  
Figure-of-Merit (FoM) 0.882923\*  
Total number of peaks 497  
Peaks in range 497  
Peaks matched 494  
Intensity scale factor 0.60\*  
Space group P -1  
Crystal system triclinic (anorthic)

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Unit cell a= 8.1796 Å b= 12.8747 Å c= 14.1720 Å α= 93.134° β= 115.885° γ= 91.236°  
I/c 0.54  
Calc. density 2.760 g/cm<sup>3</sup>  
Reference Angel R. J., Carpenter M. A., Finger L. W., "Structural variation associated with compositional variation and order-disorder behavior in anorthite-rich feldspars sample from Monte Somma", *American Mineralogist* **75**, 150-162 (1990)

**B: Rankinite (20.1 %)**

Formula sum Ca<sub>3</sub> O<sub>7</sub> Si<sub>2</sub>  
Entry number 96-901-2094  
Figure-of-Merit (FoM) 0.865150  
Total number of peaks 498  
Peaks in range 498  
Peaks matched 498  
Intensity scale factor 0.36  
Space group P 1 21/a 1  
Crystal system monoclinic  
Unit cell a= 10.6000 Å b= 8.9200 Å c= 7.8900 Å β= 119.600°  
I/c 0.50  
Calc. density 2.953 g/cm<sup>3</sup>  
Reference Kusachi I., Henmi C., Kawahara A., Henmi K., "The structure of rankinite", *Mineralogical Journal* **8**, 38-47 (1975)

**C: Dmitryivanovite (12.9 %)\***

Formula sum Al<sub>2</sub> Ca O<sub>4</sub>  
Entry number 96-901-3918  
Figure-of-Merit (FoM) 0.868973\*  
Total number of peaks 498  
Peaks in range 498  
Peaks matched 498  
Intensity scale factor 0.39\*  
Space group P 1 21/c 1  
Crystal system monoclinic  
Unit cell a= 7.9719 Å b= 8.6284 Å c= 10.2628 Å β= 94.801°  
I/c 0.84  
Calc. density 2.985 g/cm<sup>3</sup>  
Reference Lazic B., Kahlenberg V., Konzett J., "Structural studies on a stuffed framework high pressure polymorph of CaAl<sub>2</sub>O<sub>4</sub>", *Zeitschrift für Kristallographie* **222**, 690-695 (2007)

**D: Pyroxferroite (11.0 %)\***

Formula sum Ca<sub>0.94</sub> Fe<sub>6.06</sub> O<sub>21</sub> Si<sub>7</sub>  
Entry number 96-901-2890  
Figure-of-Merit (FoM) 0.863306\*  
Total number of peaks 496  
Peaks in range 496  
Peaks matched 495

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Intensity scale factor 0.35<sup>\*</sup>  
 Space group P -1  
 Crystal system triclinic (anorthic)  
 Unit cell a= 6.6213 Å b= 7.5506 Å c= 17.3806 Å α= 114.267° β= 82.684 ° γ= 94.576 °  
 I/lc 0.89  
 Calc. density 3.843 g/cm<sup>3</sup>  
 Reference Burnham C. W., "The crystal structure of pyroxferroite from Mare Tranquillitatis", Proceedings of the Second Lunar Science Conference 1, 47-57 (1971)

**E: Sanidine (9.7 %)**<sup>\*</sup>

Formula sum Al K O8 Si3  
 Entry number 96-901-7455  
 Figure-of-Merit (FoM) 0.819768<sup>\*</sup>  
 Total number of peaks 293  
 Peaks in range 293  
 Peaks matched 293  
 Intensity scale factor 0.26<sup>\*</sup>  
 Space group C 1 2/m 1  
 Crystal system monoclinic  
 Unit cell a= 8.5460 Å b= 13.0330 Å c= 7.1760 Å β= 115.970 °  
 I/lc 0.73  
 Calc. density 2.573 g/cm<sup>3</sup>  
 Reference Gering E., "Silizium/Aluminium-Ordnung und Kristallperfektion von SanidinenNote: Sample SANN, T = 1050 C, X-ray diffraction", Dissertation Kernforschungszentrum Karlsruhe 1, 1-97 (1985)

**F: Titanite (5.9 %)**<sup>\*</sup>

Formula sum Ca O5 Si Ti  
 Entry number 96-900-2443  
 Figure-of-Merit (FoM) 0.834370<sup>\*</sup>  
 Total number of peaks 500  
 Peaks in range 296  
 Peaks matched 293

Intensity scale factor 0.34<sup>\*</sup>  
 Space group P 1 21/a 1  
 Crystal system monoclinic  
 Unit cell a= 7.0187 Å b= 8.6965 Å c= 6.5243 Å β= 113.594 °  
 I/lc 1.58  
 Calc. density 3.568 g/cm<sup>3</sup>  
 Reference Kunz M., Arlt T., Stolz J., "In situ powder diffraction study of titanite (CaTiOSiO4) at high pressure and high temperatureSample", American Mineralogist 85, 1465-1473 (2000)

**G: Laihunite (5.5 %)**<sup>\*</sup>

Formula sum Fe4.74 O12 Si3  
 Entry number 96-900-1036  
 Figure-of-Merit (FoM) 0.856798<sup>\*</sup>  
 Total number of peaks 497  
 Peaks in range 497  
 Peaks matched 496  
 Intensity scale factor 0.28<sup>\*</sup>  
 Space group P 21/b 1 1  
 Crystal system monoclinic  
 Unit cell a= 4.8050 Å b= 10.1890 Å c= 17.4030 Å α= 91.000°  
 I/lc 1.40  
 Calc. density 4.218 g/cm<sup>3</sup>  
 Reference Shen B., Tamada O., Kitamura M., Morimoto N., "Superstructure of laihunite-3M (Ca<sub>40</sub>Fe<sub>80</sub>Fe<sub>80</sub>SiO<sub>4</sub>)Sample: SuperstructureFe1B-y coordinate changed by Tamada (Aug, 2001)", American Mineralogist 71, 1455-1460 (1986)

**H: Tridymite (4.1 %)**<sup>\*</sup>

Formula sum O2 Si  
 Entry number 96-901-3494  
 Figure-of-Merit (FoM) 0.840580<sup>\*</sup>  
 Total number of peaks 500  
 Peaks in range 500  
 Peaks matched 499  
 Intensity scale factor 0.22<sup>\*</sup>  
 Space group P 21 21 21  
 Crystal system orthorhombic  
 Unit cell a= 26.1630 Å b= 4.9870 Å c= 8.1990 Å  
 I/lc 1.51  
 Calc. density 2.238 g/cm<sup>3</sup>  
 Reference Hirose T., Kihara K., Okuno M., Fujinami S., Shinoda K., "X-ray, DTA and Raman studies of monoclinic tridymite and its highertemperature orthorhombic modification with varying temperature.Note: T = 413 K", Journal of Mineralogical and Petrological Sciences 100, 55-69 (2005)

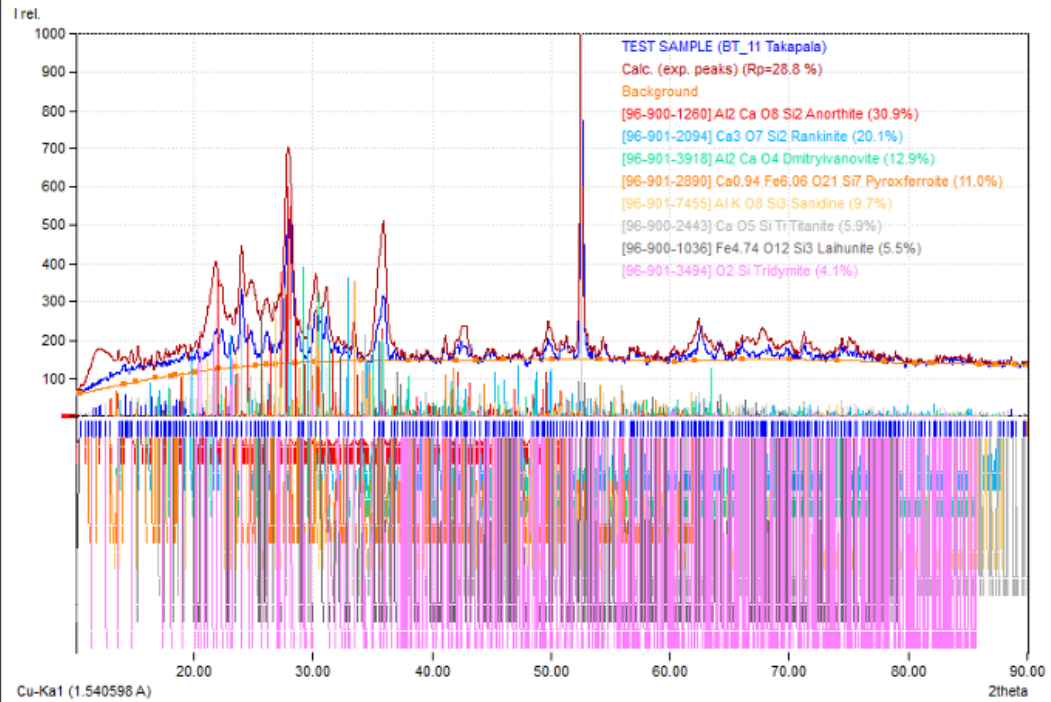
(<sup>\*</sup>)2theta values have been shifted internally for the calculation of the amounts, the intensity scaling factors as well as the figure-of-merit (FoM), due to the active search-match option 'Automatic zero point adaption'.

Profile area	Counts	Amount
Overall diffraction profile	700228	100.00%
Background radiation	576699	82.36%
Diffraction peaks	123529	17.64%
Peak area belonging to selected phases	104771	14.96%
Peak area of phase A (Anorthite)	27380	3.91%
Peak area of phase B (Rankinite)	23321	3.33%
Peak area of phase C (Dmitryivanovite)	12788	1.83%
Peak area of phase D (Pyroxferroite)	11077	1.58%
Peak area of phase E (Sanidine)	9497	1.36%
Peak area of phase F (Titanite)	6079	0.87%
Peak area of phase G (Lahunite)	8732	1.25%
Peak area of phase H (Tridymite)	5898	0.84%
Unidentified peak area	18758	2.68%

### Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	4894	100.00%
Peak intensity belonging to selected phases	4814	98.36%
Unidentified peak intensity	80	1.64%

### Diffraction Pattern Graphics



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## HASIL XRF

SAMPLE ANALYSIS REPORT  
 ARL QUANT'X EDXRF ANALYZER

THERMO FISHER SCIENTIFIC  
 UNIQUANT(TM) STANDARDLESS METHOD

C:\UQed\USER\Quant'X\Job\JOB.323 2022-08-12  
 BT1

Quant'X Rh end window 50kV  
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 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	47.39	0.60
Fe	22.33	0.28
Ca	15.23	0.27
Al	5.25	1.02
K	4.81	0.23
Ti	2.58	0.10
Sr	0.926	0.046
Px	0.49	0.12
Mn	0.359	0.058
Zr	0.214	0.056
Ba	0.185	0.040
Nb	0.0686	0.0055
Zn	0.048	0.016
Mo	0.0419	0.0083
In	0.0229	0.0012
Sn	0.0180	0.0021
Ru	0.0164	0.0041
Sb	0.0133	0.0032
Rh	0.0106	0.0040

ARL QUANT'X EDXRF ANALYZER

UNIQUANT(TM) STANDARDLESS METHOD

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 BT2

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 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 18000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	52.94	0.63
Fe	17.90	0.22
K	8.99	0.24
Ca	7.82	0.33
Al	7.27	0.97
Ti	1.62	0.20
Mn	1.05	0.06
Sr	0.766	0.038
Px	0.58	0.10
Ba	0.508	0.042
Zr	0.189	0.050
Rb	0.127	0.019
Zn	0.064	0.017
Nb	0.0595	0.0053
Mo	0.0396	0.0075
In	0.0183	0.0012
Sn	0.0177	0.0021
Ru	0.0161	0.0038
Sb	0.0124	0.0033
Rh	0.0093	0.0037

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 BT3

Quant'X Rh end window 50kv  
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 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	48.74	0.56
Fe	19.79	0.23
Ca	15.34	0.32
K	6.52	0.27
Al	4.97	0.94
Ti	1.94	0.16
Sr	0.800	0.040
Px	0.67	0.10
Mn	0.464	0.054
Ba	0.274	0.048
Zr	0.200	0.050
Nb	0.0802	0.0054
Rb	0.056	0.016
Mo	0.0518	0.0081
In	0.0268	0.0014
Sn	0.0224	0.0024
Ru	0.0222	0.0043
Sb	0.0168	0.0038
Rh	0.0124	0.0042

C:\UQed\USER\Quant'X\Job\JOB.320 2022-08-12  
 BT4

Quant'X Rh end window 50kv  
 C:\UQed\USER\Quant'X\Appl\AnySampleAir.kap 2008-06-13  
 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	49.94	0.57
Fe	18.18	0.21
Ca	13.14	0.32
K	7.75	0.26
Al	6.02	0.92
Ti	1.95	0.10
Sr	0.972	0.048
Px	0.78	0.11
Mn	0.500	0.051
Ba	0.278	0.045
Zr	0.223	0.057
Rb	0.079	0.016
Nb	0.0747	0.0050
Mo	0.0449	0.0081
In	0.0241	0.0012
Sn	0.0188	0.0022
Ru	0.0175	0.0039
Sb	0.0128	0.0034
Rh	0.0111	0.0038

SAMPLE ANALYSIS REPORT  
 ARL QUANT'X EDXRF ANALYZER

THERMO FISHER SCIENTIFIC  
 UNIQUANT(TM) STANDARDLESS METHOD

C:\UQed\USER\Quant'X\Job\JOB.327 2022-08-12  
 BT5

Quant'X Rh end window 50kv  
 C:\UQed\USER\Quant'X\Appl\AnySampleAir.kap 2008-06-13  
 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	52.28	1.58
Fe	16.32	0.50
Ca	12.13	0.37
Mg	5.52	2.49
K	5.32	0.22
Al	4.25	0.92
Ti	2.13	0.07
Sr	0.907	0.048
Mn	0.405	0.051
Px	0.35	0.11
Ba	0.122	0.036
Zr	0.112	0.056
Nb	0.0501	0.0043
Mo	0.0331	0.0055
In	0.0150	0.0009
Sn	0.0138	0.0017
Ru	0.0138	0.0032
Sb	0.0102	0.0026
Rh	0.0084	0.0031

SAMPLE ANALYSIS REPORT  
 ARL QUANT'X EDXRF ANALYZER

THERMO FISHER SCIENTIFIC  
 UNIQUANT(TM) STANDARDLESS METHOD

C:\UQed\USER\Quant'X\Job\JOB.341 2022-08-29  
 JLN#Lembanna

Quant'X Rh end window 50kv  
 C:\UQed\USER\Quant'X\Appl\AnySampleAir.kap 2008-06-13  
 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	34.26	0.51
Fe	32.22	0.40
Al	15.90	0.94
Ca	11.05	0.16
Ti	3.19	0.18
Px	1.47	0.11
Mn	0.706	0.079
K	0.55	0.17
Sr	0.224	0.011
Zr	0.188	0.022
Ni	0.081	0.023
Nb	0.0601	0.0040
Mo	0.0328	0.0066
Sn	0.0166	0.0017
In	0.0147	0.0009
Ru	0.0129	0.0031
Sb	0.0114	0.0026
Rh	0.0088	0.0029

SAMPLE ANALYSIS REPORT  
 ARL QUANT'X EDXRF ANALYZER

THERMO FISHER SCIENTIFIC  
 UNIQUANT(TM) STANDARDLESS METHOD

C:\UQed\USER\Quant'X\Job\JOB.325 2022-08-12  
 KebUn

Quant'X Rh end window 50kv  
 C:\UQed\USER\Quant'X\App1\AnySampleAir.kap 2008-06-13  
 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 18000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Fe	33.88	0.46
Si	32.57	0.54
Al	15.60	1.05
Ca	9.74	0.17
Ti	3.69	0.10
Px	1.80	0.12
K	1.22	0.17
Mn	0.753	0.085
Zr	0.254	0.025
Sr	0.203	0.013
Nb	0.0922	0.0046
Mo	0.0510	0.0080
Zn	0.051	0.017
Sn	0.0228	0.0022
In	0.0226	0.0013
Ru	0.0226	0.0033
Sb	0.0172	0.0034
Rh	0.0170	0.0031

SAMPLE ANALYSIS REPORT  
 ARL QUANT'X EDXRF ANALYZER

THERMO FISHER SCIENTIFIC  
 UNIQUANT(TM) STANDARDLESS METHOD

C:\UQed\USER\Quant'X\Job\JOB.321 2022-08-12  
 Pos#1b1#Bawakaraeng

Quant'X Rh end window 50kv  
 C:\UQed\USER\Quant'X\App1\AnySampleAir.kap 2008-06-13  
 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	41.66	0.52
Fe	25.99	0.30
Ca	13.62	0.18
Al	11.61	0.89
Ti	2.90	0.10
K	1.48	0.18
Px	0.990	0.100
Mn	0.642	0.066
Sr	0.532	0.026
Ba	0.221	0.040
Zr	0.159	0.036
Nb	0.0726	0.0050
Mo	0.0450	0.0069
In	0.0237	0.0013
Sn	0.0196	0.0023
Ru	0.0162	0.0039
Sb	0.0133	0.0035
Rh	0.0112	0.0038

SAMPLE ANALYSIS REPORT  
 ARL QUANT'X EDXRF ANALYZER

THERMO FISHER SCIENTIFIC  
 UNIQUANT(TM) STANDARDLESS METHOD

C:\UQed\USER\Quant'X\Job\JOB.328 2022-08-12  
 Pos1#Bawakaraeng

Quant'X Rh end window 50kV  
 C:\UQed\USER\Quant'X\Appl\AnySampleAir.kap 2008-06-13  
 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	47.91	0.65
Fe	20.37	0.27
Al	9.95	1.05
K	9.10	0.24
Ca	7.23	0.32
Ti	2.53	0.11
Px	0.97	0.13
Sr	0.655	0.033
Mn	0.463	0.056
Ba	0.276	0.044
Zr	0.230	0.044
Nb	0.0917	0.0046
Rb	0.067	0.019
Mo	0.0482	0.0074
Ru	0.0235	0.0032
In	0.0226	0.0014
Sn	0.0206	0.0024
Sb	0.0176	0.0036
Rh	0.0174	0.0030

SAMPLE ANALYSIS REPORT  
 ARL QUANT'X EDXRF ANALYZER

THERMO FISHER SCIENTIFIC  
 UNIQUANT(TM) STANDARDLESS METHOD

C:\UQed\USER\Quant'X\Job\JOB.326 2022-08-12  
 Takapala

Quant'X Rh end window 50kV  
 C:\UQed\USER\Quant'X\Appl\AnySampleAir.kap 2008-06-13  
 Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
 X-ray path = Air Film type = No supporting film  
 Case number = 0 All known  
 Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
 KnownConc = 0 %  
 Rest = 0 % Viewed Mass = 1000.00 mg  
 Dil/Sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
Si	44.53	0.51
Fe	23.34	0.26
Ca	17.25	0.26
K	4.91	0.23
Al	4.87	0.91
Ti	2.45	0.10
Sr	0.853	0.042
Mn	0.649	0.058
Px	0.501	0.094
Ba	0.296	0.048
Zr	0.148	0.051
Nb	0.0691	0.0052
Mo	0.0449	0.0069
In	0.0239	0.0013
Sn	0.0210	0.0024
Ru	0.0177	0.0041
Sb	0.0170	0.0036
Rh	0.0106	0.0040

C:\UQed\USER\Quant'X\Job\JOB.324 2022-08-12  
JembatanMerah

Quant'X Rh end window 50kV  
C:\UQed\USER\Quant'X\Appl\AnySampleAir.kap 2008-06-13  
Calculated as : Elements Matrix (Shape & ImpFc) : 1|Teflon  
X-ray path = Air Film type = No supporting film  
Case number = 0 All known  
Eff.Diam. = 13.0 mm Eff.Area = 132.7 mm2  
KnownConc = 0 %  
Rest = 0 % Viewed Mass = 1000.00 mg  
Dil/sample = 0 Sample Height = 5.00 mm

El	m/m%	StdErr
--	-----	-----
Si	42.07	0.51
Fe	25.97	0.29
Ca	17.20	0.20
Al	7.74	0.92
Ti	2.19	0.18
K	1.37	0.20
Px	1.09	0.10
Sr	0.847	0.042
Mn	0.646	0.067
Ba	0.210	0.039
Cr	0.156	0.068
Zr	0.145	0.050
Nb	0.0715	0.0037
Ni	0.068	0.022
Mo	0.0466	0.0055
Rb	0.046	0.018
Zn	0.036	0.013
Ru	0.0211	0.0028
In	0.0201	0.0012