**Refinement Report – Sample D**

**Global R-Values**

Rexp : 4.36 Rwp : 15.53 Rp : 11.72 GOF : 3.56

Rexp`: 7.78 Rwp`: 27.72 Rp` : 24.29 DW : 0.24

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**Quantitative Analysis - Rietveld**

Phase 1 : muscovite\_icdd\_04-015-8226 13.177 %

Phase 2 : "kaolinite \_bish\_icdd\_00-014-0164" 28.380 %

Phase 3 : quartz\_icdd\_00-046-1045 38.445 %

Phase 4 : microcline\_icdd\_00-019-0926 17.669 %

Phase 5 : albite\_icdd\_00-019-1184 2.331 %

**Background**

Chebychev polynomial, Coefficient 0 298.6996

1 -202.3374

2 75.17596

3 -50.1301

4 14.72841

5 -29.46906

**Instrument**

Primary radius (mm) 200.5

Secondary radius (mm) 200.5

Linear PSD 2Th angular range (°) 4

FDS angle (°) 0.3

Beam spill, sample length (mm) 20

Intensity corrected

Full Axial Convolution

Filament length (mm) 12

Sample length (mm) 15

Receiving Slit length (mm) 12

Primary Sollers (°) 2.5

Secondary Sollers (°) 2.5

**Corrections**

Specimen displacement -0.1528813

LP Factor 0

Absorption (1/cm) 21.11445

**Miscellaneous**

Start X 5

**Structure 1**

Phase name muscovite\_icdd\_04-015-8226

R-Bragg 0.000

Spacegroup 15

Scale 5.23198e-005

Cell Mass 1606.311

Cell Volume (Å^3) 932.19470

Wt% - Rietveld 13.177

Double-Voigt|Approach

Cry size Lorentzian 35.2

k: 1 LVol-IB (nm) 22.425

k: 0.89 LVol-FWHM (nm) 31.350

Crystal Linear Absorption Coeff. (1/cm) 180.651

Crystal Density (g/cm^3) 2.861

Preferred Orientation (Dir 1 : 0 0 1) 0.6630148

Lattice parameters

a (Å) 5.1800028

b (Å) 9.0092505

c (Å) 20.0750110

beta (°) 95.72

Site Np x y z Atom Occ Beq

O\_1 8 0.74930 0.31190 0.15780 O 1 1.364

O\_2 8 0.24770 0.36840 0.16880 O 1 1.12

O\_3 8 0.41980 0.09290 0.16830 O 1 1.263

O\_4 8 0.38640 0.25140 0.05345 O 1 1

O\_5 8 0.96110 0.44280 0.05344 O 1 0.6483

O\_6 8 0.95600 0.06280 0.05033 O 0.925 0.9666

O\_7 8 0.95600 0.06280 0.05033 O 0.055 0.9666

F\_1 8 0.95600 0.06280 0.05033 F 0.02 0.9666

Si\_1 8 0.45230 0.25823 0.13538 Si 0.753 0.4673

Al\_1 8 0.45230 0.25823 0.13538 Al 0.247 0.4673

Si\_2 8 0.96500 0.42943 0.13534 Si 0.753 0.4458

Al\_2 8 0.96500 0.42943 0.13534 Al 0.247 0.4458

Al\_3 4 0.75000 0.25000 0.00000 Al 0.0896 1.24

Fe\_1 4 0.75000 0.25000 0.00000 Fe 0.0057 1.24

Mg\_1 4 0.75000 0.25000 0.00000 Mg 0.0033 1.24

Ti\_1 4 0.75000 0.25000 0.00000 Ti 0.0014 1.24

Al\_4 8 0.24960 0.08351 -0.00001 Al 0.896 0.8226

Fe\_2 8 0.24960 0.08351 -0.00001 Fe 0.057 0.8226

Mg\_2 8 0.24960 0.08351 -0.00001 Mg 0.033 0.8226

Ti\_2 8 0.24960 0.08351 -0.00001 Ti 0.014 0.8226

K\_1 4 0.00000 0.09830 0.25000 K 0.9398 1.886

Na\_1 4 0.00000 0.09830 0.25000 Na 0.04018 1.886

**Structure 2**

Phase name kaolinite \_bish\_icdd\_00-014-0164

R-Bragg 0.000

Spacegroup C1

Scale 1.00597e-003

Cell Mass 508.257

Cell Volume (Å^3) 330.01683

Wt% - Rietveld 28.380

Double-Voigt|Approach

Cry size Lorentzian 17.9

Cry size Gaussian 9999.6

k: 1 LVol-IB (nm) 11.385

k: 0.89 LVol-FWHM (nm) 15.911

Strain

Strain L 1

Strain G 0.832958

e0 0.00325

Crystal Linear Absorption Coeff. (1/cm) 113.582

Crystal Density (g/cm^3) 2.557

Preferred Orientation (Dir 1 : 0 0 1) 0.8802152

(Dir 2 : 0 2 0) 1

Fraction of Dir 1 1

Lattice parameters

a (Å) 5.1545803

b (Å) 8.9000000

c (Å) 7.4500000

alpha (°) 92.3

beta (°) 104.8984

gamma (°) 89.20729

Site Np x y z Atom Occ Beq

s1 2 0.99420 0.33930 0.09090 SI+4 1 0.44

s2 2 0.50640 0.16650 0.09130 SI+4 1 0.44

s3 2 0.29710 0.49570 0.47210 AL+3 1 0.83

s4 2 0.79260 0.33000 0.46990 AL+3 1 0.83

s5 2 0.05010 0.35390 0.31700 O-2 1 0.71

s6 2 0.12140 0.66040 0.31750 O-2 1 0.71

s7 2 0.00000 0.50000 0.00000 O-2 1 0.71

s8 2 0.20850 0.23050 0.02470 O-2 1 0.71

s9 2 0.20120 0.76570 0.00320 O-2 1 0.71

s10 2 0.05100 0.96980 0.32200 O-2 1 0.9

s11 2 0.96490 0.16650 0.60510 O-2 1 0.9

s12 2 0.03480 0.47690 0.60800 O-2 1 0.9

s13 2 0.03340 0.85700 0.60940 O-2 1 0.9

**Structure 3**

Phase name quartz\_icdd\_00-046-1045

R-Bragg 0.000

Spacegroup 154

Scale 1.12122e-002

Cell Mass 180.253

Cell Volume (Å^3) 113.09960

Wt% - Rietveld 38.445

Crystal Linear Absorption Coeff. (1/cm) 137.275

Crystal Density (g/cm^3) 2.646

Lattice parameters

a (Å) 4.9148289

c (Å) 5.4064681

Site Np x y z Atom Occ Beq

Si\_1 3 0.47230 0.00000 0.66667 Si 1 0.5953

O\_1 6 0.41600 0.26580 0.78810 O 1 1.379

**Structure 4**

Phase name microcline\_icdd\_00-019-0926

R-Bragg 0.000

Spacegroup C-1

Scale 1.30786e-004

Cell Mass 1113.326

Cell Volume (Å^3) 721.46567

Wt% - Rietveld 17.669

Crystal Linear Absorption Coeff. (1/cm) 186.773

Crystal Density (g/cm^3) 2.562

Preferred Orientation (Dir 1 : 0 0 1) 0.9239721

(Dir 2 : 0 0 2) 0.4636586

Fraction of Dir 1 0.8140687

Lattice parameters

a (Å) 8.5819883

b (Å) 12.9576309

c (Å) 7.2135852

alpha (°) 90.53672

beta (°) 115.8344

gamma (°) 87.84943

Site Np x y z Atom Occ Beq

s1 4 0.28310 -0.00670 0.13600 K+1 1 1.35

s2 4 0.00960 0.18800 0.21790 AL+3 0.9 0.6

SI+4 0.1 0.6

s3 4 0.00980 0.81910 0.23270 AL+3 0.03 0.61

SI+4 0.97 0.61

s4 4 0.71170 0.12000 0.34000 AL+3 0.07 0.56

SI+4 0.93 0.56

s5 4 0.70670 0.88580 0.34950 SI+4 1 0.54

s6 4 0.00070 0.14480 -0.01790 O-2 1 1.11

s7 4 0.63610 0.00530 0.28620 O-2 1 0.58

s8 4 0.82180 0.14760 0.22000 O-2 1 1.14

s9 4 0.83070 0.85680 0.24350 O-2 1 1.42

s10 4 0.03470 0.31880 0.25640 O-2 1 0.67

s11 4 0.03820 0.69550 0.26460 O-2 1 0.74

s12 4 0.19000 0.12280 0.40550 O-2 1 1.14

s13 4 0.17540 0.87450 0.40910 O-2 1 1.31

**Structure 5**

Phase name albite\_icdd\_00-019-1184

R-Bragg 0.000

Spacegroup C-1

Scale 1.97891e-005

Cell Mass 1048.495

Cell Volume (Å^3) 667.82851

Wt% - Rietveld 2.331

Crystal Linear Absorption Coeff. (1/cm) 127.114

Crystal Density (g/cm^3) 2.607

Lattice parameters

a (Å) 8.1406098

b (Å) 12.7875911

c (Å) 7.1999998

alpha (°) 94.42275

beta (°) 116.6566

gamma (°) 87.58801

Site Np x y z Atom Occ Beq

s1 4 0.26750 0.98020 0.15100 NA+1 0.45 6

s2 4 0.26530 0.00000 0.13850 NA+1 0.55 6

s3 4 0.00950 0.16800 0.20750 SI+4 0.09 0.2

AL+3 0.91 0.2

s4 4 0.00530 0.82070 0.23800 SI+4 0.95 0.2

AL+3 0.05 0.2

s5 4 0.69100 0.11000 0.31050 SI+4 0.91 0.2

AL+3 0.09 0.2

s6 4 0.67970 0.88180 0.35950 SI+4 0.96 0.2

AL+3 0.04 0.2

s7 4 0.00650 0.12830 0.96780 O-2 1 0.15

s8 4 0.59050 0.99620 0.27850 O-2 1 0.15

s9 4 0.81690 0.10700 0.19430 O-2 1 0.35

s10 4 0.81910 0.85250 0.26120 O-2 1 0.35

s11 4 0.00950 0.30110 0.26800 O-2 1 0.35

s12 4 0.02470 0.69360 0.22950 O-2 1 0.15

s13 4 0.20850 0.10870 0.38850 O-2 1 0.15

s14 4 0.18440 0.86740 0.43450 O-2 1 0.15