**Analysis Report – Sigma Standard sample**

**Global R-Values**

Rexp : 4.08 Rwp : 13.26 Rp : 9.98 GOF : 3.25

Rexp`: 7.82 Rwp`: 25.42 Rp` : 21.08 DW : 0.20

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**Quantitative Analysis - Rietveld**

Phase 1 : quartz\_icdd\_00-046-1045 1.798 %

Phase 2 : "kaolinite \_bish\_icdd\_00-014-0164" 84.167 %

Phase 3 : muscovite\_icdd\_04-015-8226 4.230 %

Phase 4 : calcite\_magnesian\_3\_santos\_et\_al\_2017 0.981 %

Phase 5 : dolomite\_ii\_nonstoich\_santos\_et\_al\_2017 1.403 %

Phase 6 : gibbsite\_icdd\_04-014-4442 6.002 %

Phase 7 : montmorillonite\_cod\_9002779 0.612 %

Phase 8 : alunite\_cod\_9012350 0.807 %

**Background**

Chebychev polynomial, Coefficient 0 365.0906

1 -243.3442

2 140.6326

3 -77.79043

4 54.23276

5 -36.38484

**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 0.2118072

LP Factor 0

Absorption (1/cm) 6.182138

**Miscellaneous**

Start X 5

**Structure 1**

Phase name quartz\_icdd\_00-046-1045

R-Bragg 0.000

Spacegroup 154

Scale 6.50502e-004

Cell Mass 180.253

Cell Volume (Å^3) 110.36595

Wt% - Rietveld 1.798

Crystal Linear Absorption Coeff. (1/cm) 140.675

Crystal Density (g/cm^3) 2.712

Lattice parameters

a (Å) 4.8639078

c (Å) 5.3868368

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 2**

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

R-Bragg 0.000

Spacegroup C1

Scale 3.63845e-003

Cell Mass 508.257

Cell Volume (Å^3) 327.52750

Wt% - Rietveld 84.167

Double-Voigt|Approach

Cry size Lorentzian 12.8

Cry size Gaussian 80.4

k: 1 LVol-IB (nm) 7.985

k: 0.89 LVol-FWHM (nm) 11.064

Strain

Strain L 0.7509767

Strain G 1.499811

e0 0.00424

Crystal Linear Absorption Coeff. (1/cm) 114.445

Crystal Density (g/cm^3) 2.577

Preferred Orientation (Dir 1 : 0 0 1) 0.3896628

(Dir 2 : 0 2 0) 1

Fraction of Dir 1 0.01207662

Lattice parameters

a (Å) 5.1318406

b (Å) 8.9000000

c (Å) 7.4500000

alpha (°) 92.3

beta (°) 105.5617

gamma (°) 89.56223

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 muscovite\_icdd\_04-015-8226

R-Bragg 0.000

Spacegroup 15

Scale 2.09053e-005

Cell Mass 1606.311

Cell Volume (Å^3) 906.38984

Wt% - Rietveld 4.230

Crystal Linear Absorption Coeff. (1/cm) 185.795

Crystal Density (g/cm^3) 2.943

Preferred Orientation (Dir 1 : 0 0 1) 1

Lattice parameters

a (Å) 5.1114219

b (Å) 8.9670682

c (Å) 19.8742452

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 4**

Phase name calcite\_magnesian\_3\_santos\_et\_al\_2017

R-Bragg 0.000

Spacegroup 167

Scale 3.31271e-005

Cell Mass 590.358

Cell Volume (Å^3) 360.80089

Wt% - Rietveld 0.981

Double-Voigt|Approach

Cry size Lorentzian 32.0

k: 1 LVol-IB (nm) 20.372

k: 0.89 LVol-FWHM (nm) 28.480

Crystal Linear Absorption Coeff. (1/cm) 273.746

Crystal Density (g/cm^3) 2.717

Preferred Orientation (Dir 1 : 1 0 4) 0.5

Lattice parameters

a (Å) 4.9707753

c (Å) 16.8612090

Site Np x y z Atom Occ Beq

s1 6 0.00000 0.00000 0.00000 CA+2 0.8926 0.95

MG+2 0.1074 0.95

s2 6 0.00000 0.00000 0.25000 C 1 0.9

s3 18 0.25700 0.00000 0.25000 O 1 0.94

**Structure 5**

Phase name dolomite\_ii\_nonstoich\_santos\_et\_al\_2017

R-Bragg 3.675

Spacegroup 148

Scale 5.58904e-005

Cell Mass 557.934

Cell Volume (Å^3) 323.54142

Wt% - Rietveld 1.403

Double-Voigt|Approach

Cry size Lorentzian 32.0

k: 1 LVol-IB (nm) 20.372

k: 0.89 LVol-FWHM (nm) 28.480

Crystal Linear Absorption Coeff. (1/cm) 213.511

Crystal Density (g/cm^3) 2.864

Preferred Orientation (Dir 1 : 1 0 4) 1

Brindley correction - Spherical particles

Particle Radius (cm) 1e-005

Packing density 0.4

Mass Ab. Coefficient (cm^2/g) 74.56194464

Lattice parameters

a (Å) 4.8186800

c (Å) 16.0895200

Site Np x y z Atom Occ Beq

A 3 0.00000 0.00000 0.00000 CA+2 1 0.7

B 3 0.00000 0.00000 0.50000 MG+2 0.9 0.5

Ca+2 0.1 1

s3 6 0.00000 0.00000 0.24290 C 1 0.7

s4 18 0.24850 -0.03430 0.24390 O 1 0.8

**Structure 6**

Phase name gibbsite\_icdd\_04-014-4442

R-Bragg 0.000

Spacegroup 14

Scale 1.62184e-004

Cell Mass 624.028

Cell Volume (Å^3) 426.79590

Wt% - Rietveld 6.002

Double-Voigt|Approach

Cry size Lorentzian 148.5

k: 1 LVol-IB (nm) 94.519

k: 0.89 LVol-FWHM (nm) 132.138

Crystal Linear Absorption Coeff. (1/cm) 81.611

Crystal Density (g/cm^3) 2.428

Lattice parameters

a (Å) 8.8354032

b (Å) 5.0515314

c (Å) 9.5927176

beta (°) 94.55

Site Np x y z Atom Occ Beq

Al\_1 4 0.16788 0.52910 -0.00220 Al 1 0.548

Al\_2 4 0.33442 0.02359 -0.00236 Al 1 0.5598

O\_1 4 0.17810 0.21820 -0.11160 O 1 0.7256

O\_2 4 0.66950 0.65600 -0.10270 O 1 0.683

O\_3 4 0.49840 0.13040 -0.10450 O 1 0.7359

O\_4 4 -0.02040 0.62910 -0.10710 O 1 0.6695

O\_5 4 0.29700 0.71750 -0.10580 O 1 0.7564

O\_6 4 0.81920 0.14880 -0.10190 O 1 0.7082

H\_1 4 0.09800 0.15300 -0.12700 H 1 2.763

H\_2 4 0.59500 0.57000 -0.10300 H 1 3.237

H\_3 4 0.49800 0.10700 -0.19200 H 1 2.053

H\_4 4 -0.05600 0.77800 -0.11700 H 1 4.737

H\_5 4 0.29400 0.71800 -0.18800 H 1 2.369

H\_6 4 0.80700 0.15200 -0.18900 H 1 1.263

**Structure 7**

Phase name montmorillonite\_cod\_9002779

R-Bragg 0.000

Spacegroup P\_1

Scale 9.03337e-006

Cell Mass 756.674

Cell Volume (Å^3) 643.99254

Wt% - Rietveld 0.612

Double-Voigt|Approach

Cry size Lorentzian 10.0

Cry size Gaussian 10.0

k: 1 LVol-IB (nm) 4.490

k: 0.89 LVol-FWHM (nm) 5.425

Crystal Linear Absorption Coeff. (1/cm) 115.677

Crystal Density (g/cm^3) 1.951

Preferred Orientation (Dir 1 : 0 0 1) 1

(Dir 2 : 0 -1 3) 1

Fraction of Dir 1 0.0001

Lattice parameters

a (Å) 5.1721419

b (Å) 8.4494698

c (Å) 14.7362145

alpha (°) 90.11445

beta (°) 90.24944

gamma (°) 89.99254

Site Np x y z Atom Occ Beq

al\_1 1 0.87530 0.33300 0.22140 al 1 1.578

al\_2 1 0.87530 0.66700 0.22140 al 1 1.578

al\_3 1 0.37530 0.83300 0.22140 al 1 1.578

al\_4 1 0.37530 0.16700 0.22140 al 1 1.578

si\_1 1 0.55880 0.32900 0.04300 si 1 1.578

si\_2 1 0.55880 0.67100 0.04300 si 1 1.578

si\_3 1 0.69190 0.82900 0.39990 si 1 1.578

si\_4 1 0.69190 0.17100 0.39990 si 1 1.578

si\_5 1 0.05880 0.82900 0.04300 si 1 1.578

si\_6 1 0.05880 0.17100 0.04300 si 1 1.578

si\_7 1 0.19190 0.32900 0.39990 si 1 1.578

si\_8 1 0.19190 0.67100 0.39990 si 1 1.578

o\_1 1 0.51340 0.50000 0.00990 o 1 1.578

o\_2 1 0.82800 0.72800 0.00000 o 1 1.578

o\_3 1 0.82800 0.27200 0.00000 o 1 1.578

o\_4 1 0.49540 0.00000 0.15200 o 1 1.578

o\_5 1 0.56820 0.69100 0.14870 o 1 1.578

o\_6 1 0.57220 0.30900 0.14870 o 1 1.578

o\_7 1 0.73730 0.00000 0.43290 o 1 1.578

o\_8 1 0.42270 0.22800 0.44280 o 1 1.578

o\_9 1 0.42270 0.77200 0.44280 o 1 1.578

o\_10 1 0.75530 0.50000 0.29080 o 1 1.578

o\_11 1 0.68240 0.19100 0.29410 o 1 1.578

o\_12 1 0.67840 0.80900 0.29410 o 1 1.578

o\_13 1 0.01340 0.00000 0.00990 o 1 1.578

o\_14 1 0.32800 0.22800 0.00000 o 1 1.578

o\_15 1 0.32800 0.77200 0.00000 o 1 1.578

o\_16 1 0.99540 0.50000 0.15200 o 1 1.578

o\_17 1 0.06820 0.19100 0.14870 o 1 1.578

o\_18 1 0.07220 0.80900 0.14870 o 1 1.578

o\_19 1 0.23730 0.50000 0.43290 o 1 1.578

o\_20 1 0.92270 0.72800 0.44280 o 1 1.578

o\_21 1 0.92270 0.27200 0.44280 o 1 1.578

o\_22 1 0.25530 0.00000 0.29080 o 1 1.578

o\_23 1 0.18240 0.69100 0.29410 o 1 1.578

o\_24 1 0.17840 0.30900 0.29410 o 1 1.578

ca\_1 1 0.18930 0.00000 0.72150 ca 0.5 1.578

ca\_2 1 0.68930 0.50000 0.72150 ca 0.5 1.578

**Structure 8**

Phase name alunite\_cod\_9012350

R-Bragg 0.000

Spacegroup R\_-3\_m

Scale 6.54811e-006

Cell Mass 1252.117

Cell Volume (Å^3) 708.73430

Wt% - Rietveld 0.807

Crystal Linear Absorption Coeff. (1/cm) 178.242

Crystal Density (g/cm^3) 2.934

Lattice parameters

a (Å) 6.9197471

c (Å) 17.0911927

Site Np x y z Atom Occ Beq

k\_1 3 0.00000 0.00000 0.00000 k 0.875 0.57

al\_1 9 0.50000 0.00000 0.50000 al 1 0.69

s\_1 6 0.00000 0.00000 0.30350 s 1 0.379

o\_1 3 0.00000 0.00000 0.00000 o 0.125 0.839

o\_2 6 0.00000 0.00000 0.38670 o 1 0.858

o\_3 18 0.21910 -0.21910 0.94050 o 1 0.599

o\_4 18 0.12500 -0.12500 0.14210 o 1 0.57

h\_1 36 0.19506 0.19506 0.11278 h 1 1.53