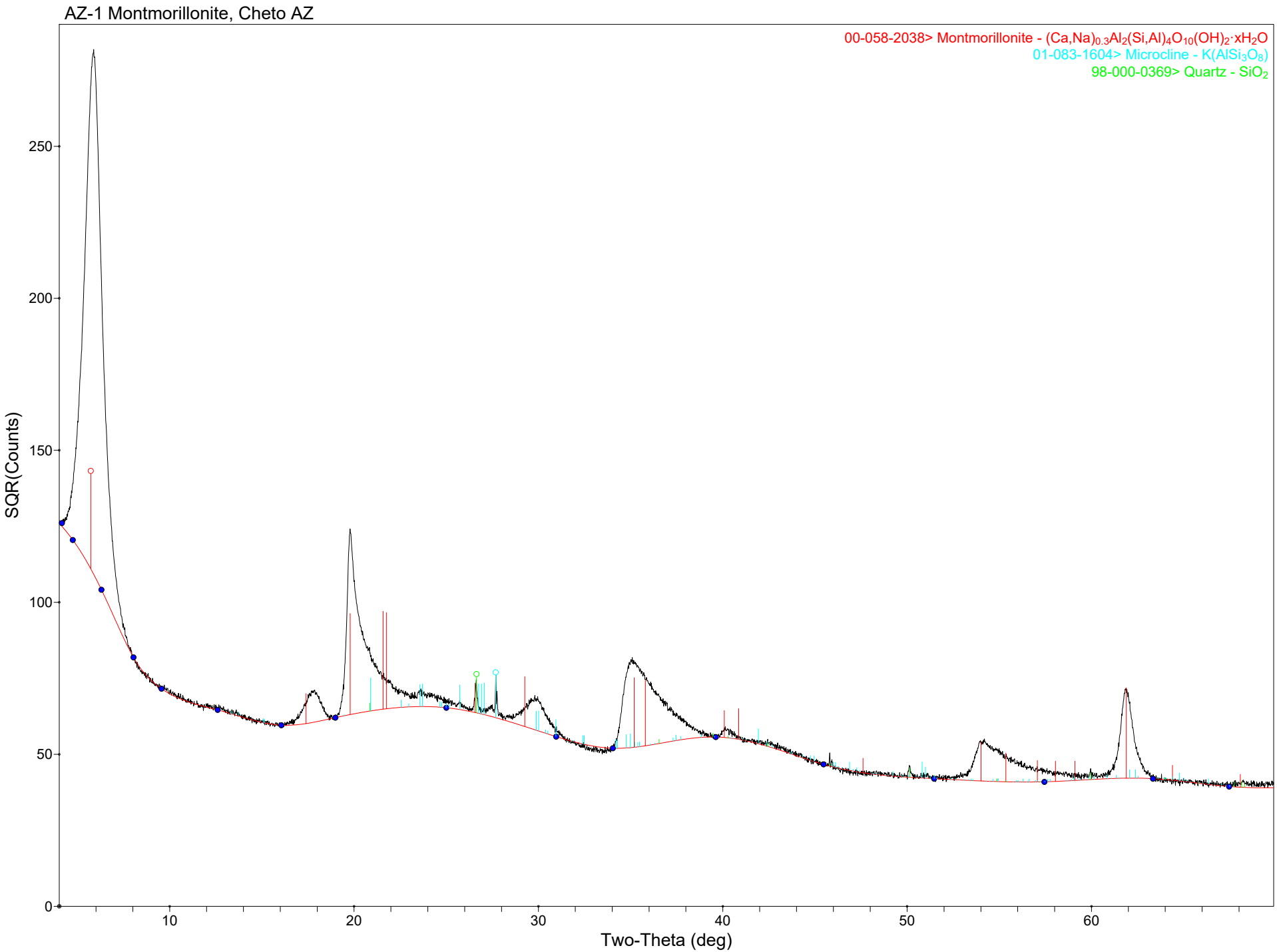

AZ-1 Montmorillonite, Cheto AZ
00-058-2038> Montmorillonite - (Ca,Na)0.3Al2(Si,Al)4O10(OH)2·xH2O
01-083-1604> Microcline - K(AlSi3O8)
98-000-0369> Quartz - SiO2
SQR(Counts)
0
50
100
150
200
250
10
20
30
40
50
60
Two-Theta (deg)

EMIT_Basalt_Weathered_Surface

FILE: [BR93-43 Weathered Basalt weathered surface.mdi]
SCAN: 3.0/149.98/0.02/1(sec), Cu, I(p)=3862, 11/23/21 10:12p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\BR93-43 Weathere...

☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering
☑ Caglioti's FWHM Function

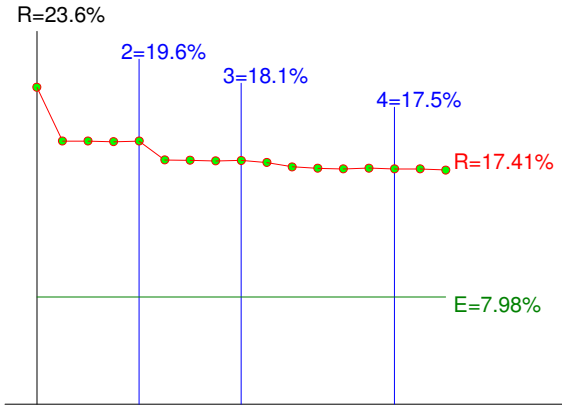
[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 72.5(deg)
☑ Zero Offset of Goniometer - 2Theta = -0.161471(0.04233)
☑ Specimen Displacement - Cos(Theta) = -0.001264(0.044097)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

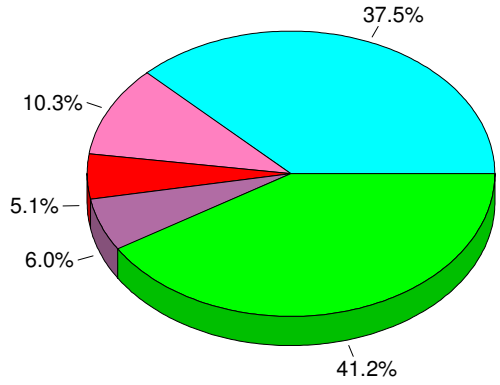
Phase ID (5)	Source	I/Ic	Wt%	#L	PC
Albite - $Na(AlSi_3O_8)$	PDF#01-089-6424	0.64(5%)	37.5 (2.3)	199	SHF(6,3)
Clinochlore IIb - $Mg_{4.54}Al_{0.97}Fe_{0.46}Mn_{0.03}(Si_{2.85}Al_{1.15}O_{10})(OH)_8$	PDF#98-000-0165	0.81(0%)	10.3 (0.5)	298	<None>
Muscovite 2M - $KAl_2[Si_3Al]O_{10}(OH)_2$	PDF#98-000-0321	0.40(0%)	5.1 (0.6)	212	<None>
Microcline - $K(AlSi_3O_8)$	PDF#98-000-0305	0.63(0%)	6.0 (0.5)	331	<None>
Quartz - SiO_2	PDF#98-000-0369	4.28(0%)	41.2 (1.1)	54	<None>

XRF(Wt%): Fe=0.5%, Mn=0.0%, K=1.3%, Si=35.6%, Al=6.5%, Mg=2.0%, Na=3.3%, O=50.6%, H=0.1%

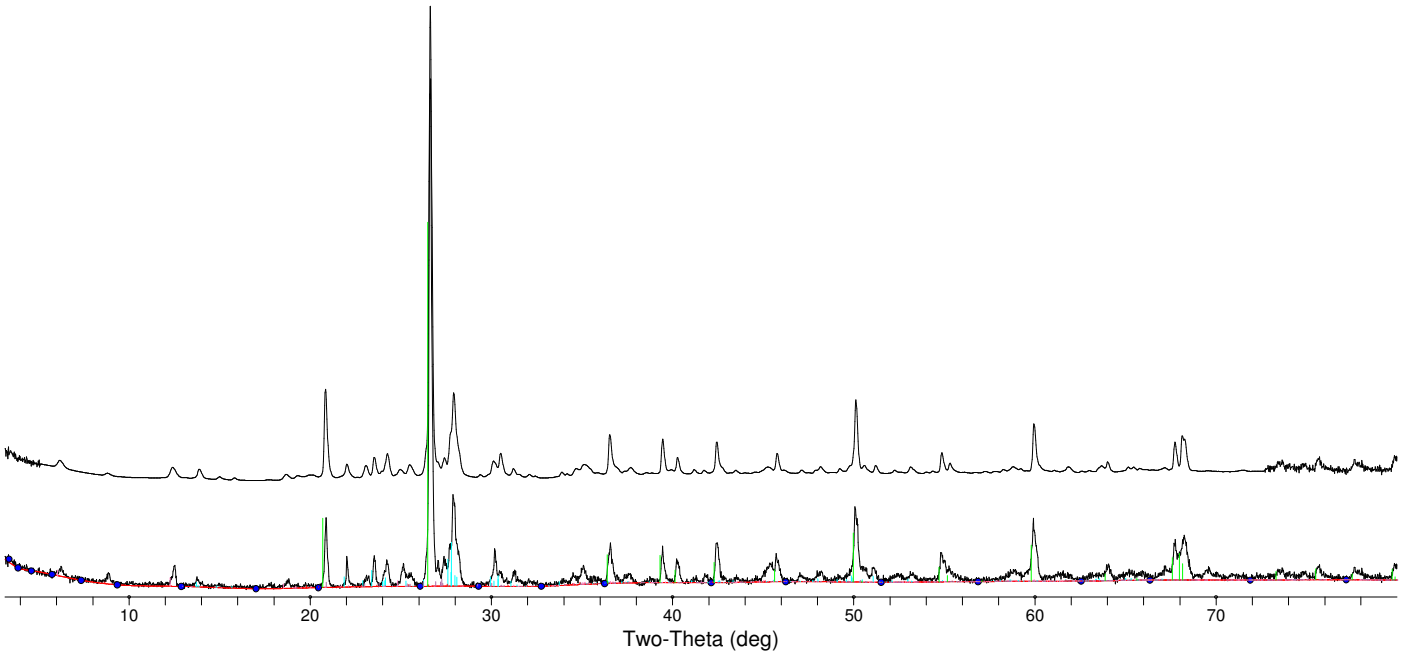
NOTE: Fitting Halted at Iteration 17(4): R=17.41% (E=7.98%, R/E=2.18, P=19, EPS=0.5)



Refinement Iterations



Wt%



EMIT-WS272 Calcite, Tunguska, Russia

FILE: [Wbsss-6196-01_EMIT_Calcite.xrdml] WS272 Calcite, Tunguska, Russia
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=113985, 08/23/21 12:54p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108005_WBSSS-6196_EMIT_Group-2\Wbsss-6196-01_EMIT_Ca...

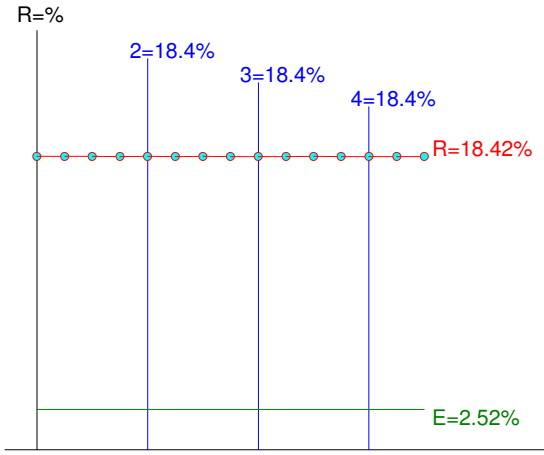
- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering
- [Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)
- ☑ Specimen Displacement - Cos(Theta) = 0.009163(0.002231)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

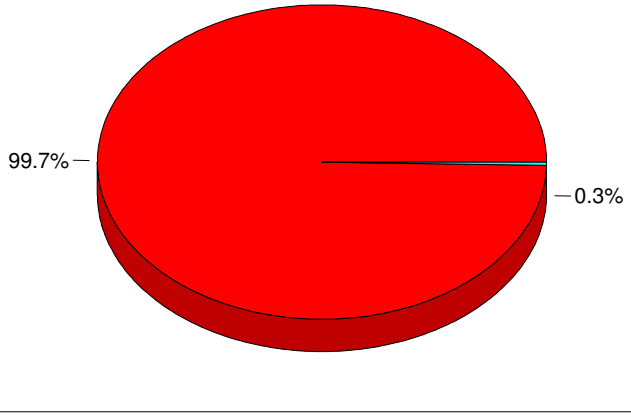
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

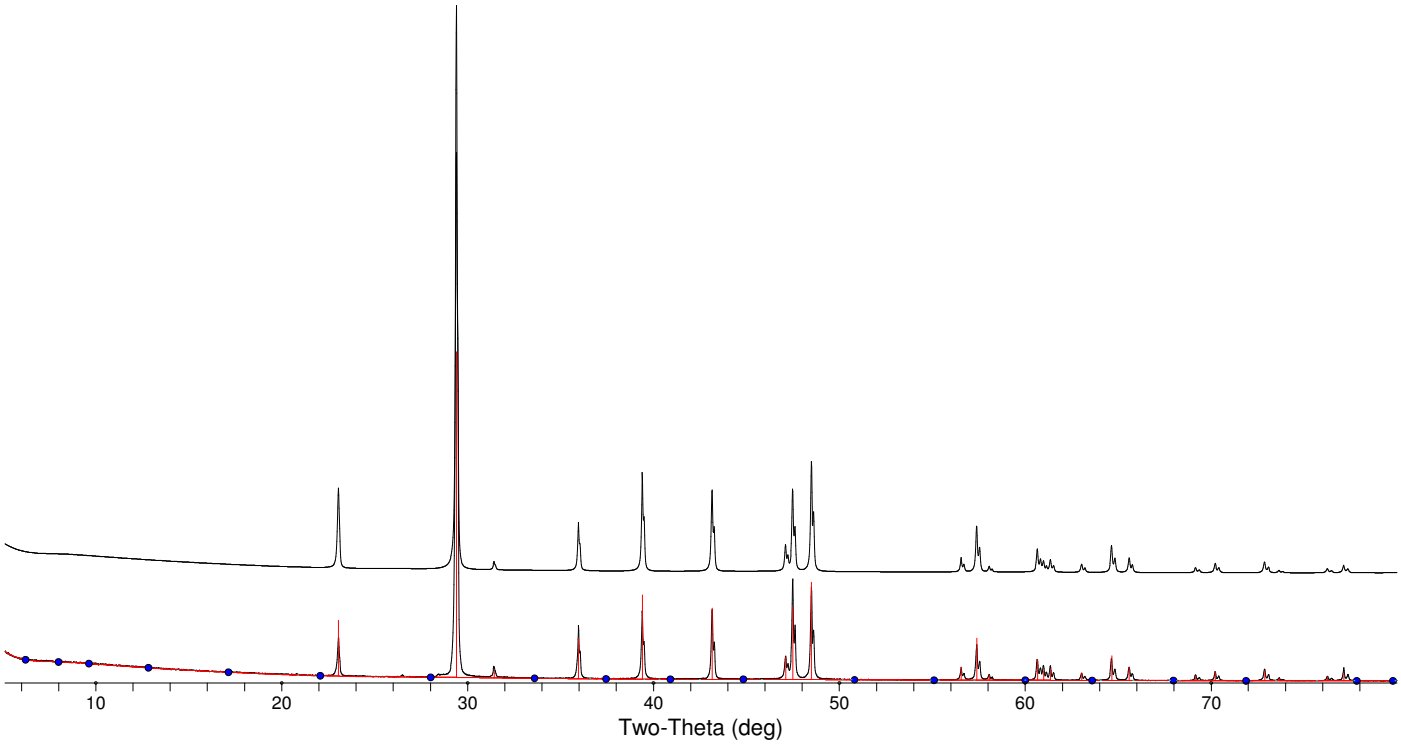
Phase ID (2)	Source	I/Ic	Wt%	#L
Calcite - $CaCO_3$	PDF#98-000-0141	2.99(0%)	99.7 (0.8)	26
Quartz - SiO_2	PDF#98-000-0369	4.22(0%)	0.3 (0.2)	68

XRF(Wt%): Ca=39.9%, Si=0.1%, O=48.0%, C=12.0%

NOTE: Fitting Halted at Iteration 15(4): R=18.42% (E=2.52%, R/E=7.3, P=14, EPS=0.5)







Chlorite plus goethite CU92-4B

FILE: [CU92-4B Chlorite plus Goethite.mdi]
SCAN: 3.0/149.98/0.02/1(sec), Cu, I(p)=3862, 11/23/21 10:11p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\CU92-4B Chlorite p...

- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering
- ☑ Caglioti's FWHM Function

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 120.0(deg)

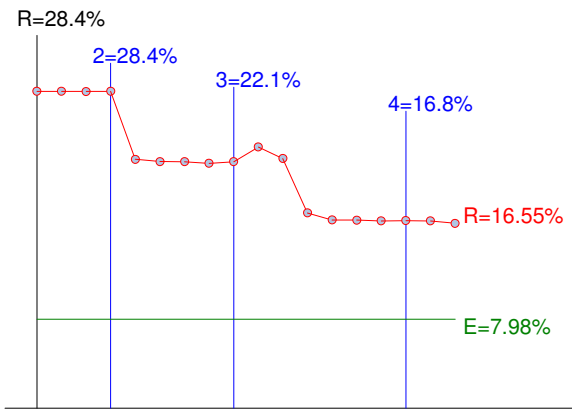
- ☑ Zero Offset of Goniometer - 2Theta = -0.057066(0.027949)
- ☑ Specimen Displacement - Cos(Theta) = -0.088652(0.029445)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

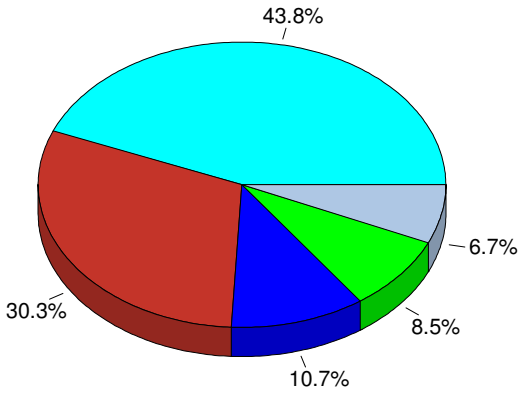
Phase ID (5)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#98-000-0369	4.27(0%)	43.8 (1.0)	154
Albite - $Na(AlSi_3O_8)$	PDF#01-089-6424	0.64(5%)	30.3 (1.8)	199
Clinochlore IIb - $Mg_{4.54}Al_{0.97}Fe_{0.46}Mn_{0.03}(Si_{2.85}Al_{1.15}O_{10})(OH)_8$	PDF#98-000-0165	0.80(0%)	10.7 (0.6)	866
Microcline - $K(AlSi_3O_8)$	PDF#98-000-0305	0.63(0%)	8.5 (0.6)	989
Muscovite 2M - $KaI_2[Si_3Al]O_{10}(OH)_2$	PDF#98-000-0321	0.40(0%)	6.7 (0.7)	697

XRF(Wt%): Fe=0.5%, Mn=0.0%, K=1.9%, Si=35.7%, Al=6.4%, Mg=2.1%, Na=2.7%, O=50.7%, H=0.2%

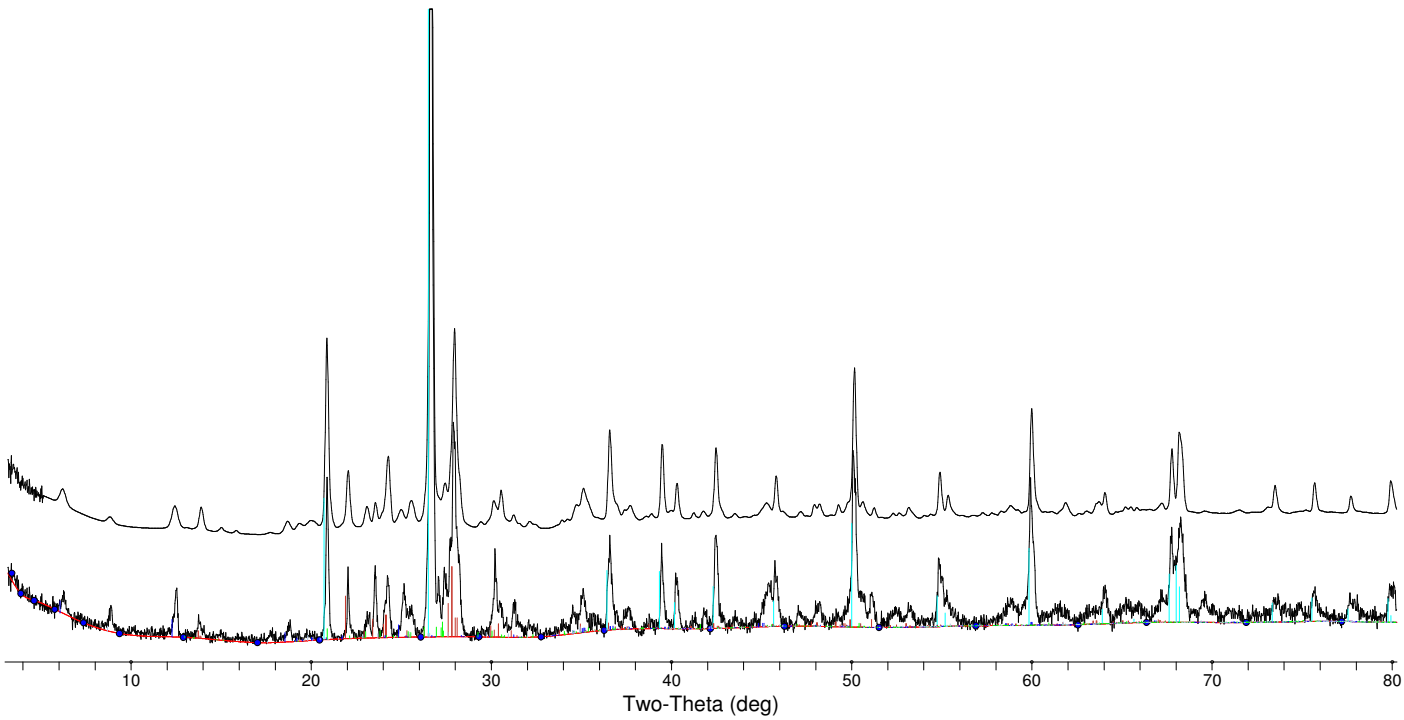
NOTE: Fitting Halted at Iteration 18(4): R=16.55% (E=7.98%, R/E=2.07, P=18, EPS=0.5)

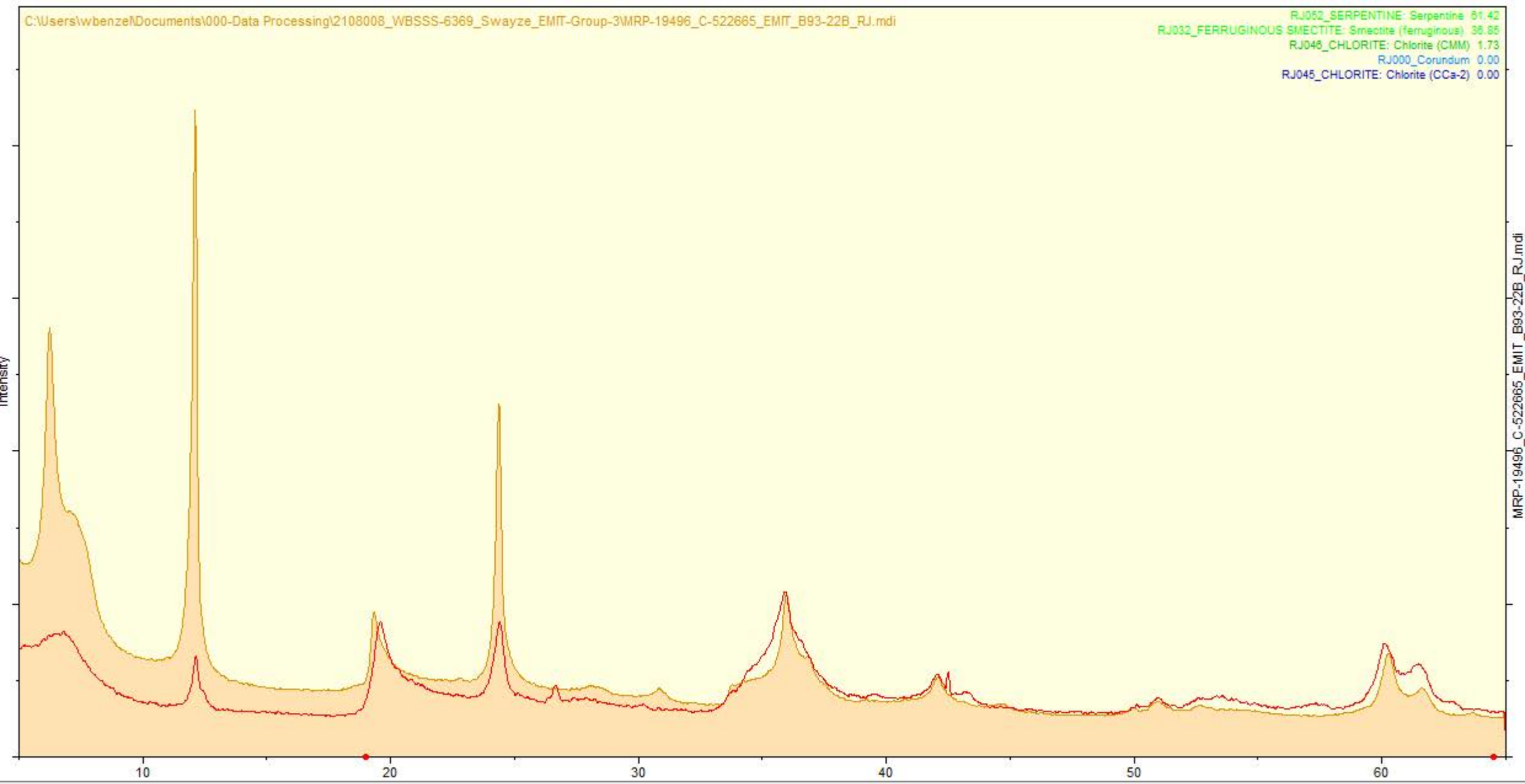


Refinement Iterations



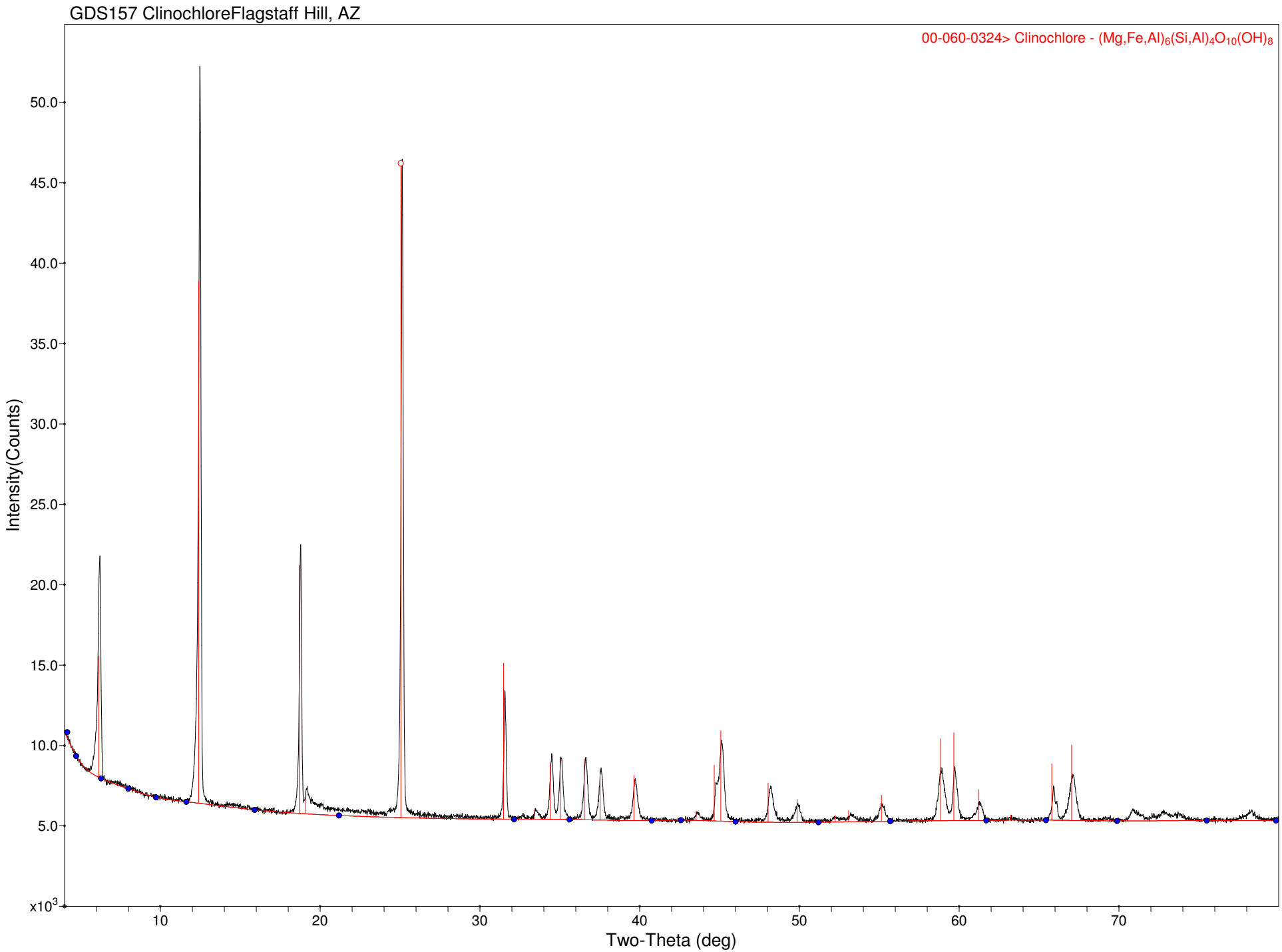
Wt%





(3) MIF [5-65] Al2O3 | 0 | 0.04 | 100 | 12 LSR cycles, Rp=16.19%, d2T=-0.06, Rwp=20.02%

#	Description	Scale	Best w[%]	d2Th	MIF	Rank
☑ 1	RJ000_Corundum	0.0000	0.00	0.00	1	0.27
☑ 52	**RJ052_SERPENTINE: Serpentine**	130.8181	61.42	-0.060	1.472	0.19
☑ 32	**RJ032_FERRUGINOUS SMECTITE: Smectite (ferr...**	94.7628	36.85	-0.060	1.726	0.74
☑ 46	**RJ046_CHLORITE: Chlorite (CMM)**	5.2943	1.73	-0.060	1.906	0.50


GDS157 ClinochloreFlagstaff Hill, AZ
00-060-0324> Clinochlore - (Mg,Fe,Al)6(Si,Al)4O10(OH)8
Intensity(Counts)
x10^3
50.0
45.0
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
10
20
30
40
50
60
70
Two-Theta (deg)

EMIT-GDS158 Clinochlore, Flagstaff Hill Area, AZ

FILE: [Wbsss-6196-03_EMIT_Clinochlore.xrdml] GDS158 Clinochlore, Flagstaff Hill Area, AZ
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=142616, 08/24/21 08:09a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108005_WBSSS-6196_EMIT_Group-2\Wbsss-6196-03_EMIT_Cl...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 72.3(deg)

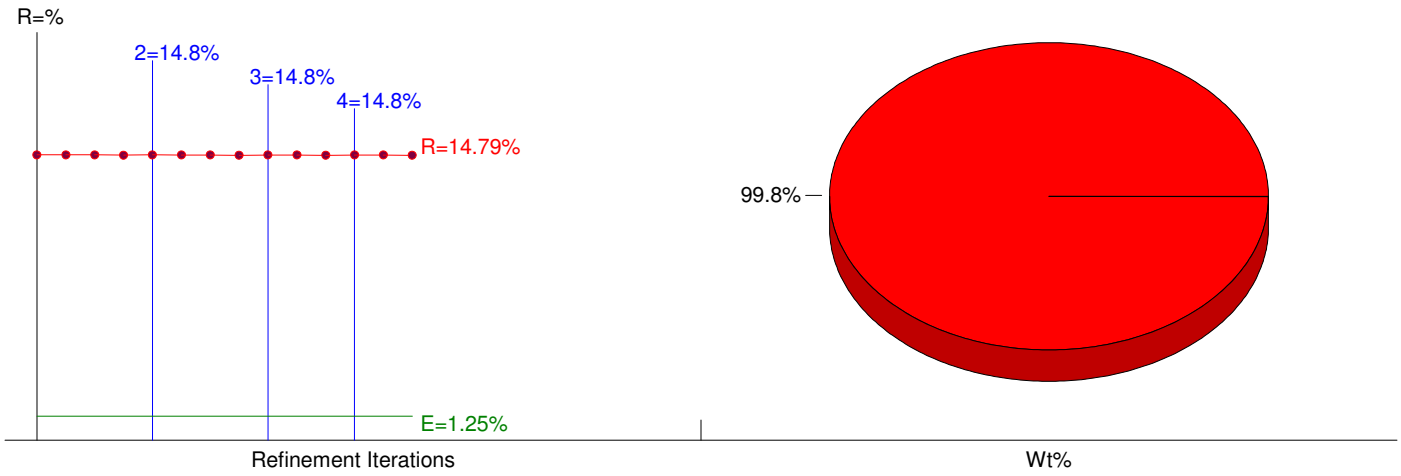
- ☑ Zero Offset of Goniometer - 2Theta = -0.785349(0.114783)
- ☑ Specimen Displacement - Cos(Theta) = 0.902275(0.112639)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

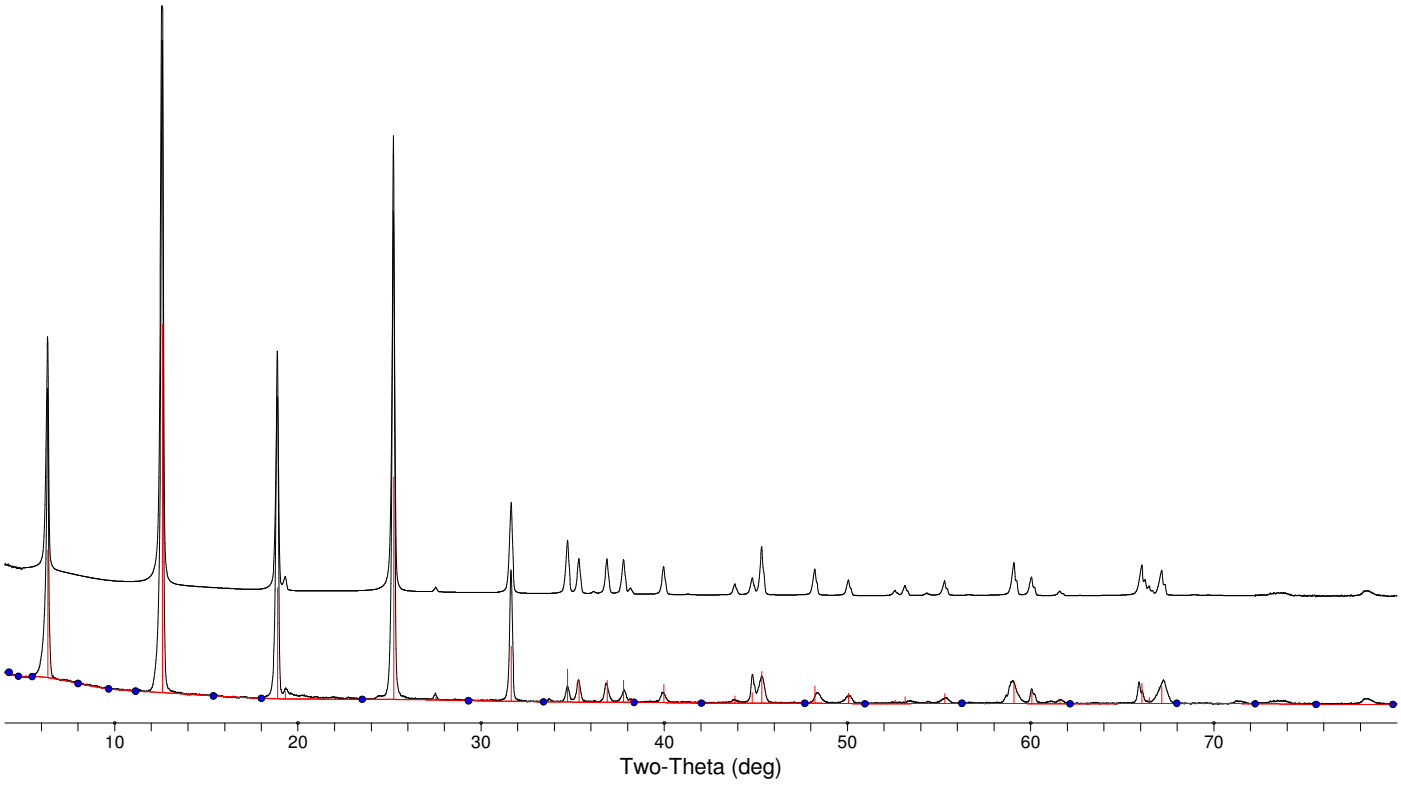
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

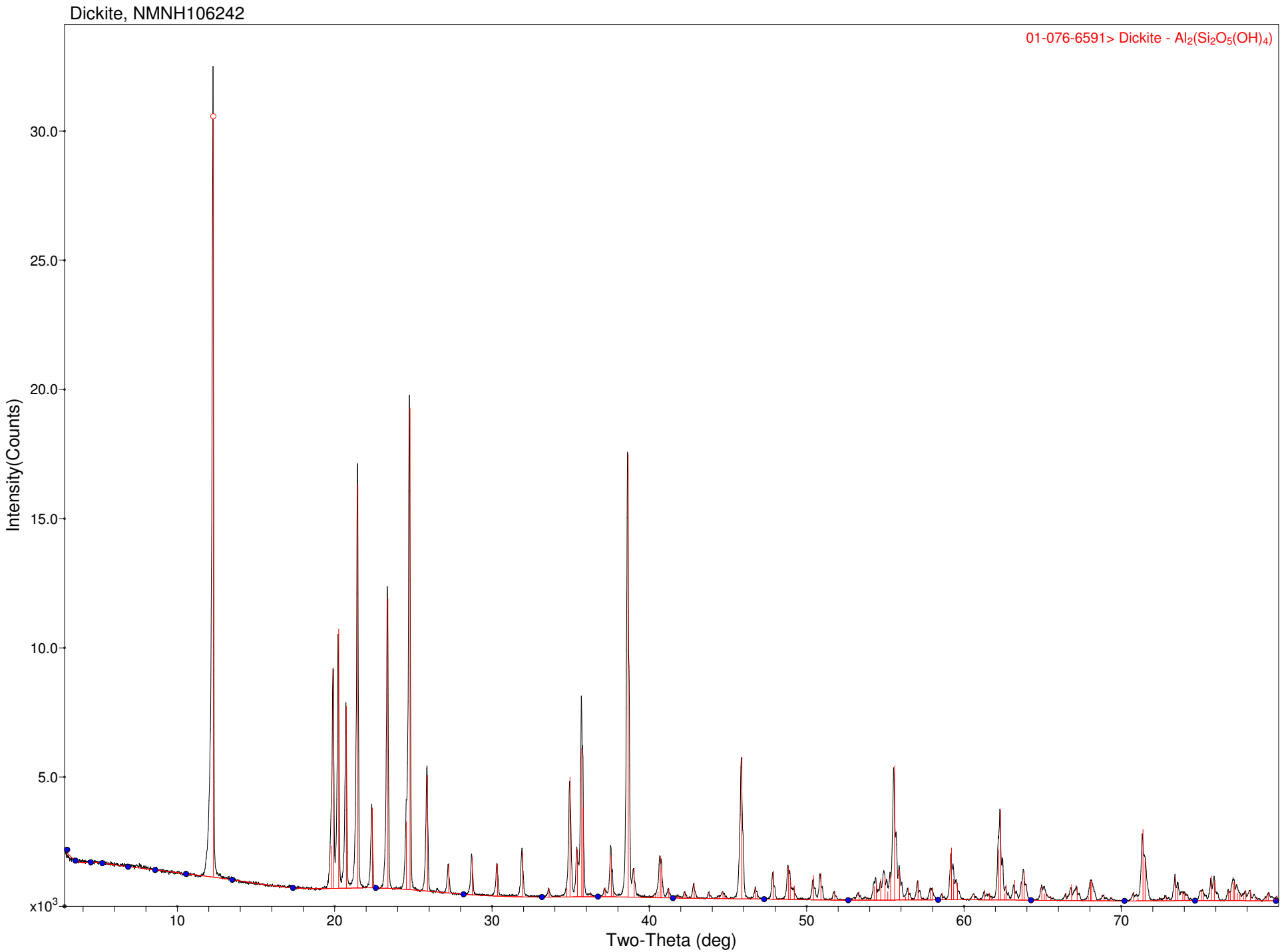
Phase ID (2)	Source	I/Ic	Wt%	#L
Clinochlore - $(Mg,Fe)_6(Si,Al)_4O_{10}(OH)_8$	PDF#00-029-0701	0.80(5%)	99.8 (7.1)	26
Rutile - TiO_2	PDF#98-000-0375	3.37(0%)	0.2 (0.0)	12

XRF(Wt%): Fe=25.9%, Ti=0.1%, Si=8.7%, Al=8.3%, Mg=11.3%, O=44.5%, H=1.2%

NOTE: Fitting Halted at Iteration 14(4): R=14.79% (E=1.25%, R/E=11.82, P=15, EPS=0.5)






Dickite, NMNH106242
01-076-6591> Dickite - Al2(Si2O5(OH)4)
Intensity(Counts)
x10^3
30.0
25.0
20.0
15.0
10.0
5.0
10
20
30
40
50
60
70
Two-Theta (deg)

Emit-HS103.3B Dolomite, Lee MA

FILE: [MRP-19177_C-522587_Dolomite.xrdml] HS103.3B Dolomite, Lee MA
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=37794, 08/25/21 01:37a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2105001 MRP-19177_Swayze_EMIT_Group-1\MRP-19177_C-522...

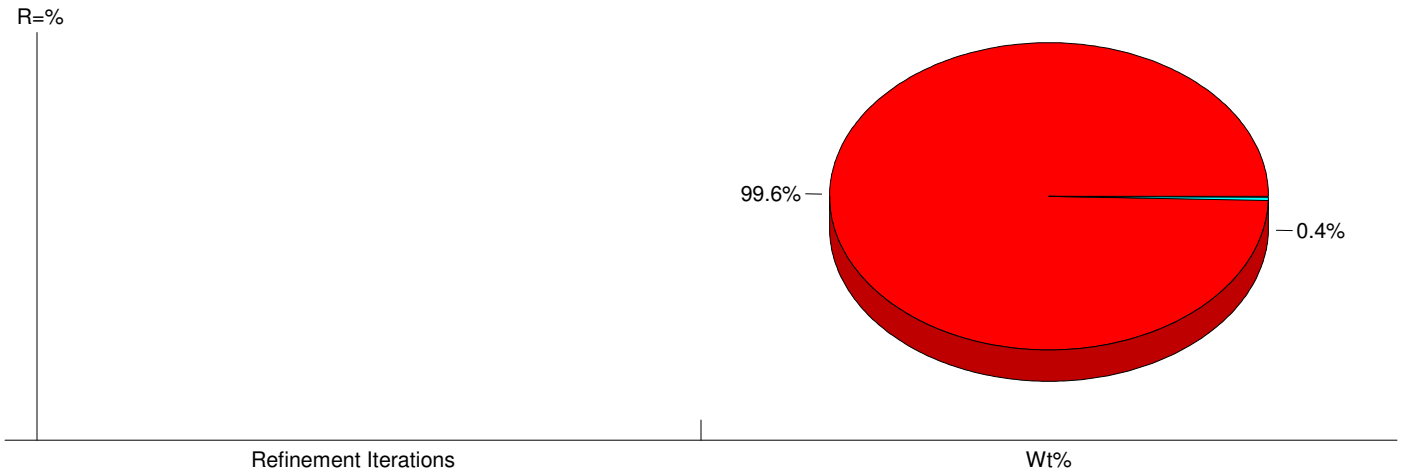
- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering
- [Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)
- ☑ Specimen Displacement - Cos(Theta) = -0.053187(0.007444)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

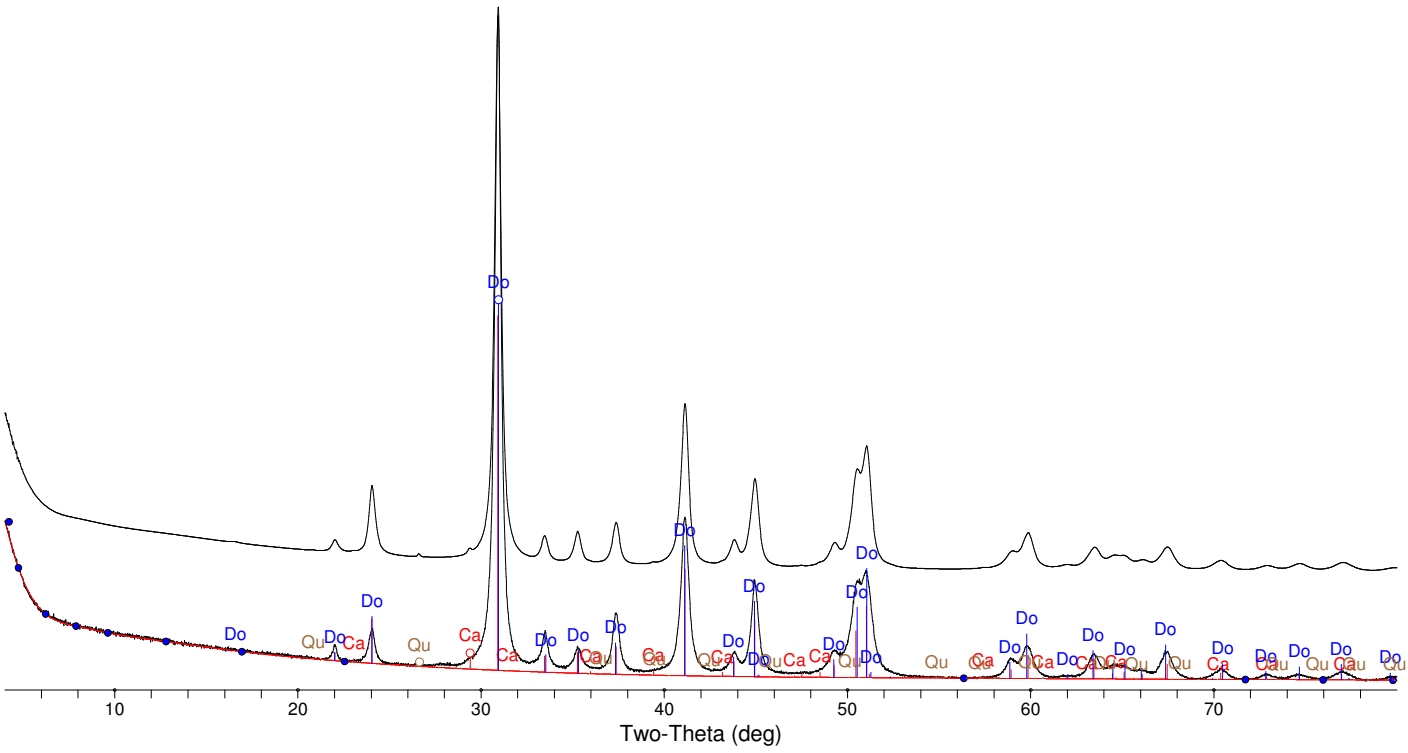
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (3)	Source	I/Ic	Wt%	#L
Dolomite - $MgCa(CO_3)_2$	PDF#98-000-0200	2.27(0%)	99.6 (0.5)	44
Calcite - $CaCO_3$	PDF#98-000-0141	3.00(0%)	0.4 (0.0)	26
Quartz - SiO_2	PDF#98-000-0369	4.24(0%)	0.1 (0.0)	68

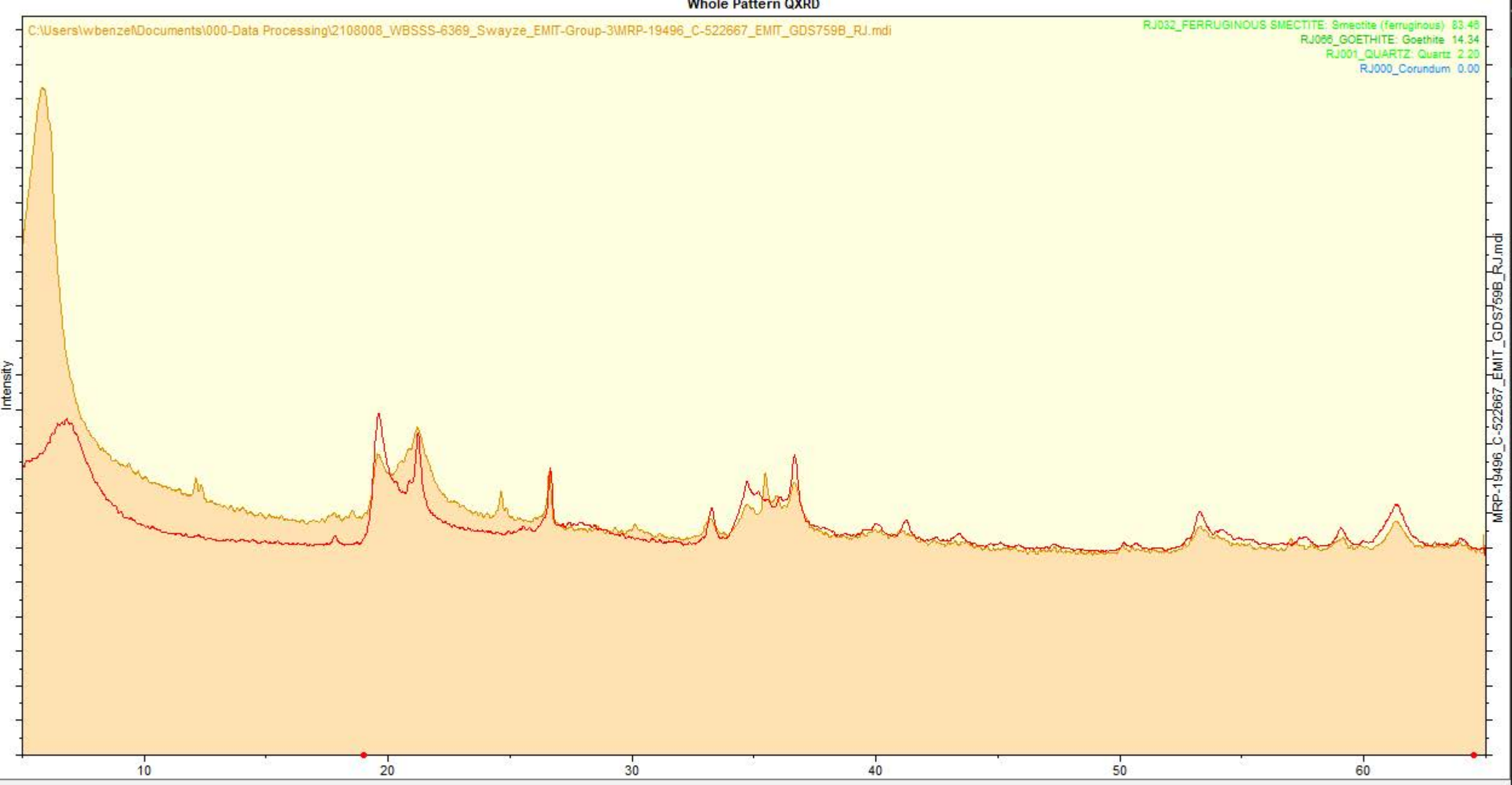
XRF(Wt%): Ca=21.8%, Si=0.0%, Mg=13.1%, O=52.0%, C=13.0%

NOTE: Fitting Halted at Iteration 0(1): R=10.93% (E=2.24%, R/E=4.88, P=12, EPS=0.5)



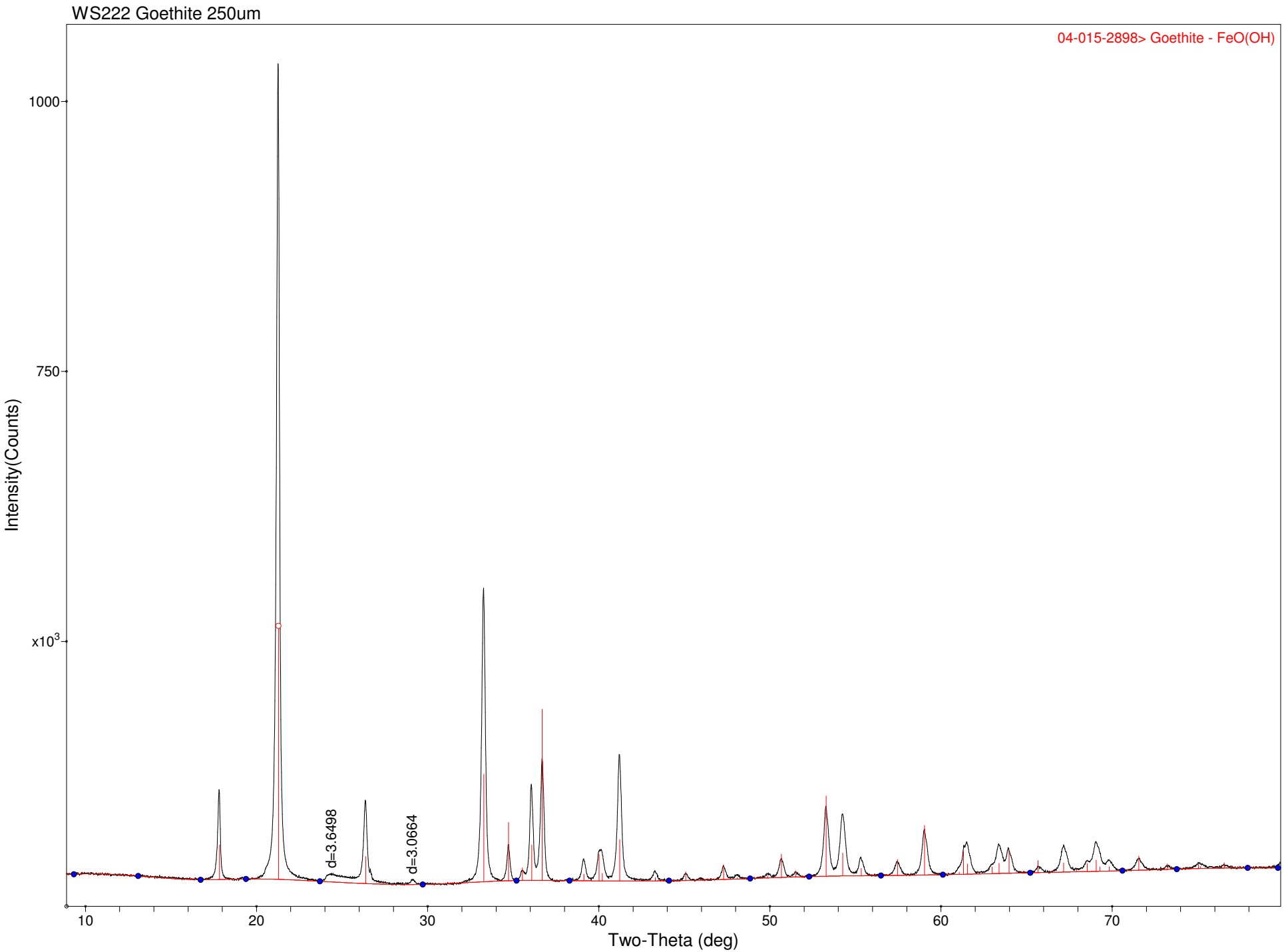


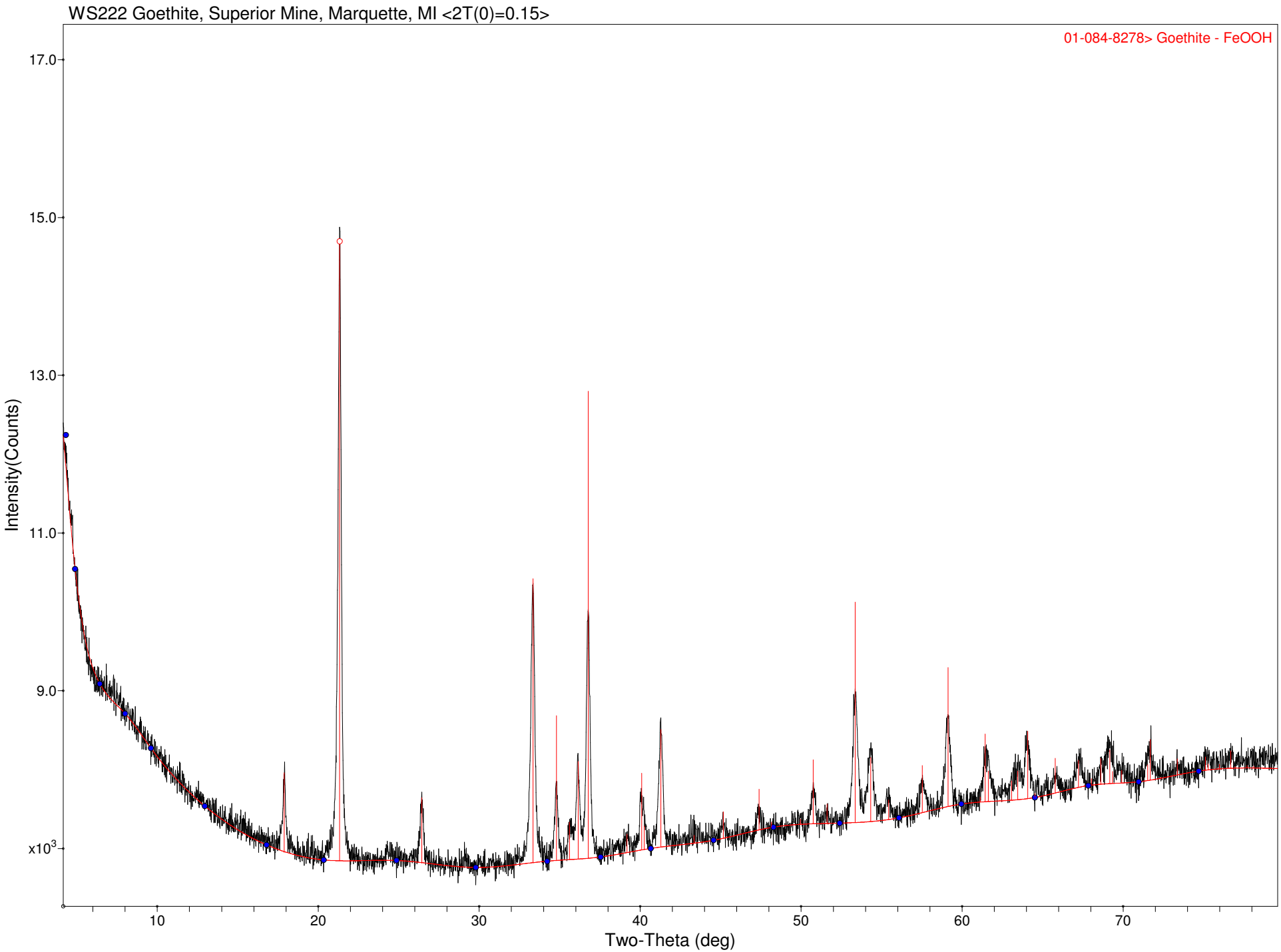
Whole Pattern QXRD

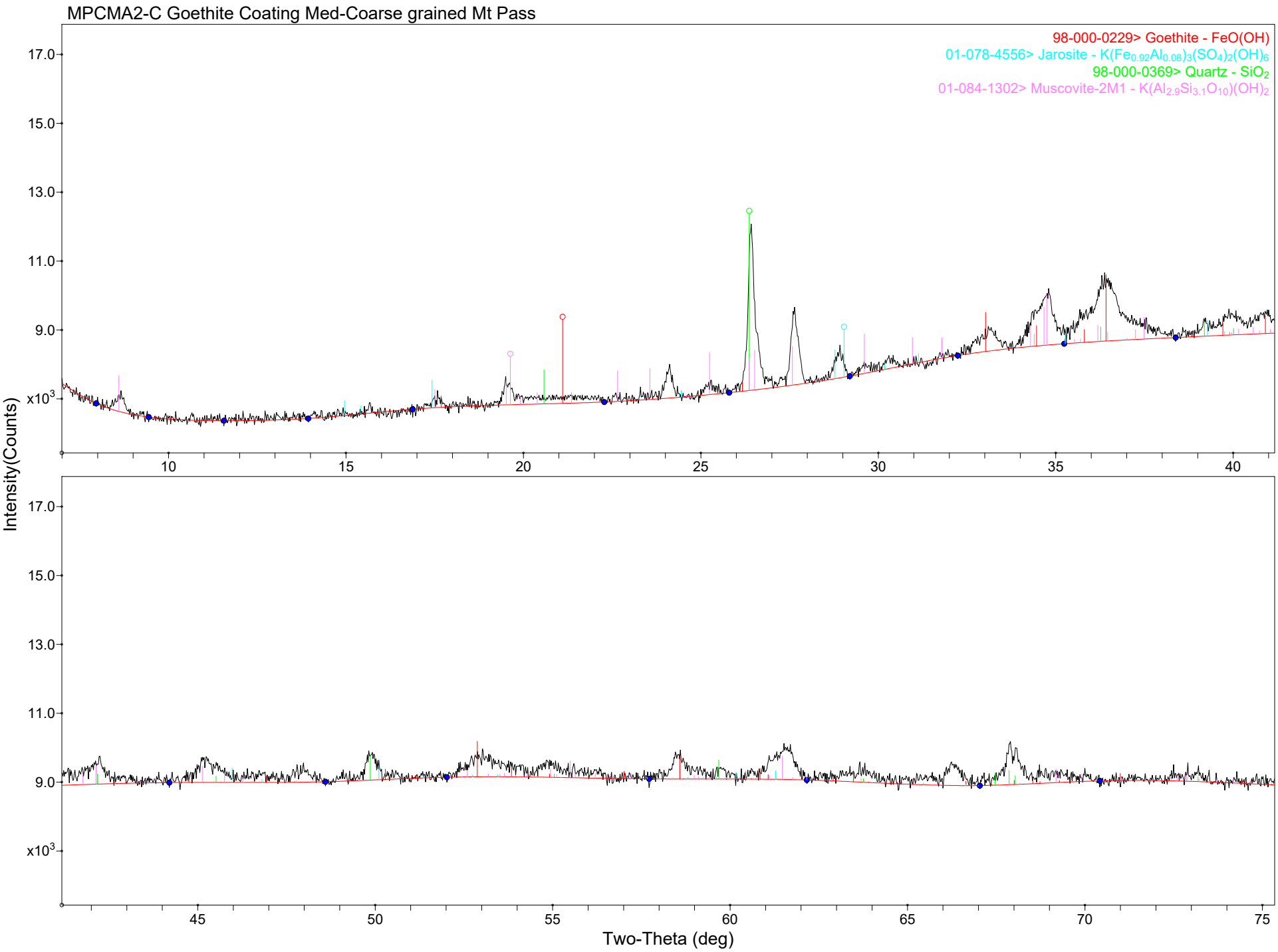


(3) MIF [5-65] Al2O3 | 0 | 0.04 | 100 | 12 LSR cycles, Rp=3.50%, d2T=-0.04, Rwp=4.74%

#	Description	Scale	Best w[%]	d2Th	MIF	Rank
☑ 1	RJ000_Corundum	0.0000	0.00	0.00	1	0.27
☑ 32	**RJ032_FERRUGINOUS SMECTITE: Smectite (ferr...**	27.6104	83.46	-0.040	1.726	0.74
☑ 66	**RJ066_GOETHITE: Goethite**	11.1389	14.34	-0.040	2.263	0.49
☑ 2	**RJ001_QUARTZ: Quartz**	0.4843	2.20	-0.040	1.654	0.29


WS222 Goethite 250um
04-015-2898> Goethite - FeO(OH)
1000
750
x10^3
Intensity(Counts)
d=3.6498
d=3.0664
10
20
30
40
50
60
70
Two-Theta (deg)


WS222 Goethite, Superior Mine, Marquette, MI <2T(0)=0.15>
01-084-8278> Goethite - FeOOH
17.0
15.0
13.0
11.0
9.0
x10^3
Intensity(Counts)
10
20
30
40
50
60
70
Two-Theta (deg)


MPCMA2-C Goethite Coating Med-Coarse grained Mt Pass
98-000-0229> Goethite - FeO(OH)
01-078-4556> Jarosite - K(Fe0.92Al0.08)3(SO4)2(OH)6
98-000-0369> Quartz - SiO2
01-084-1302> Muscovite-2M1 - K(Al2.9Si3.1O10)(OH)2
Intensity(Counts)
x10^3
17.0
15.0
13.0
11.0
9.0
10
15
20
25
30
35
40
45
50
55
60
65
70
75
Two-Theta (deg)

EMIT-HS333.3B Gypsum

FILE: [MRP-19177_C-522588_Gypsum.xrdml] HS333.3B Gypsum
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=169636, 08/25/21 02:55a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2105001 MRP-19177_Swayze_EMIT_Group-1\MRP-19177_C-522...

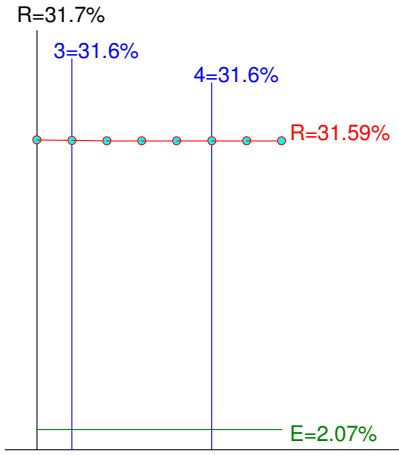
☑ K-alpha2 Peak Present
☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering
[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 77.7(deg)
☑ Specimen Displacement - Cos(Theta) = -0.002635(0.005599)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

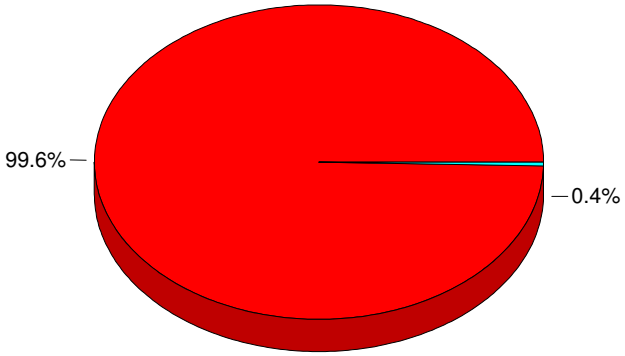
Phase ID (2)	Source	I/Ic	Wt%	#L
Gypsum - $CaSO_4 \cdot 2H_2O$	PDF#98-000-0234	1.98(0%)	99.6 (1.3)	148
Bassanite - $CaSO_4 \cdot 0.5H_2O$	PDF#98-000-0108	1.17(0%)	0.4 (0.1)	684

XRF(Wt%): Ca=23.3%, S=18.6%, O=55.7%, H=2.3%

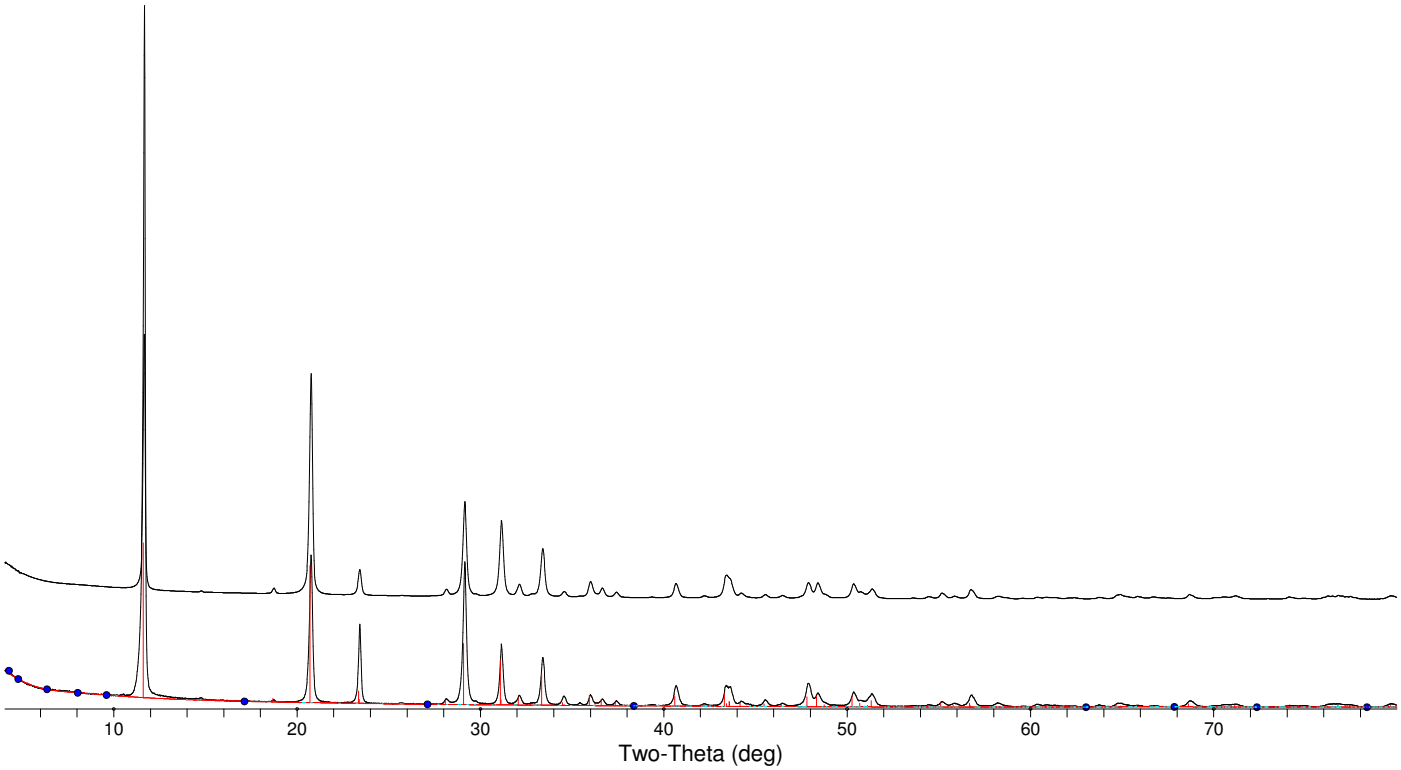
NOTE: Fitting Halted at Iteration 8(4): R=31.59% (E=2.07%, R/E=15.24, P=16, EPS=0.5)



Refinement Iterations



Wt%



EMIT-Halloysite NMNH106237

FILE: [WBSSS-6196-14_2108005-14_Halloysite.xrdml] Halloysite NMNH106237
SCAN: 3.5458/79.9999/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=6126, 08/20/21 07:08p
PROC: [WPF Control File]

☑ K-alpha2 Peak Present
☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering

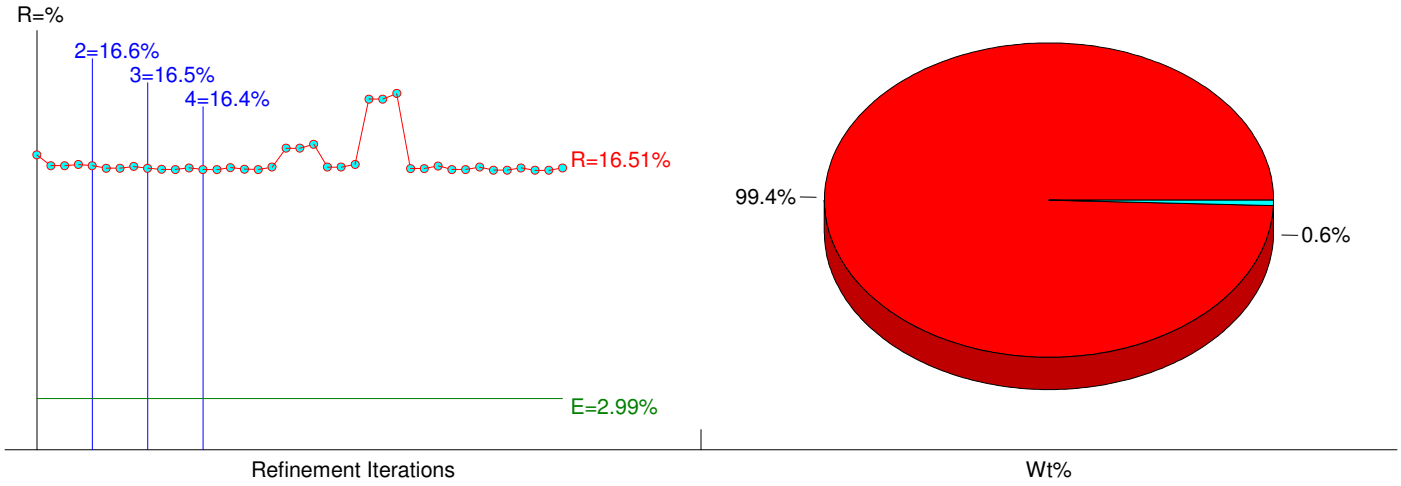
[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 78.7(deg)
☑ Specimen Displacement - Cos(Theta) = -0.085603(0.008342)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

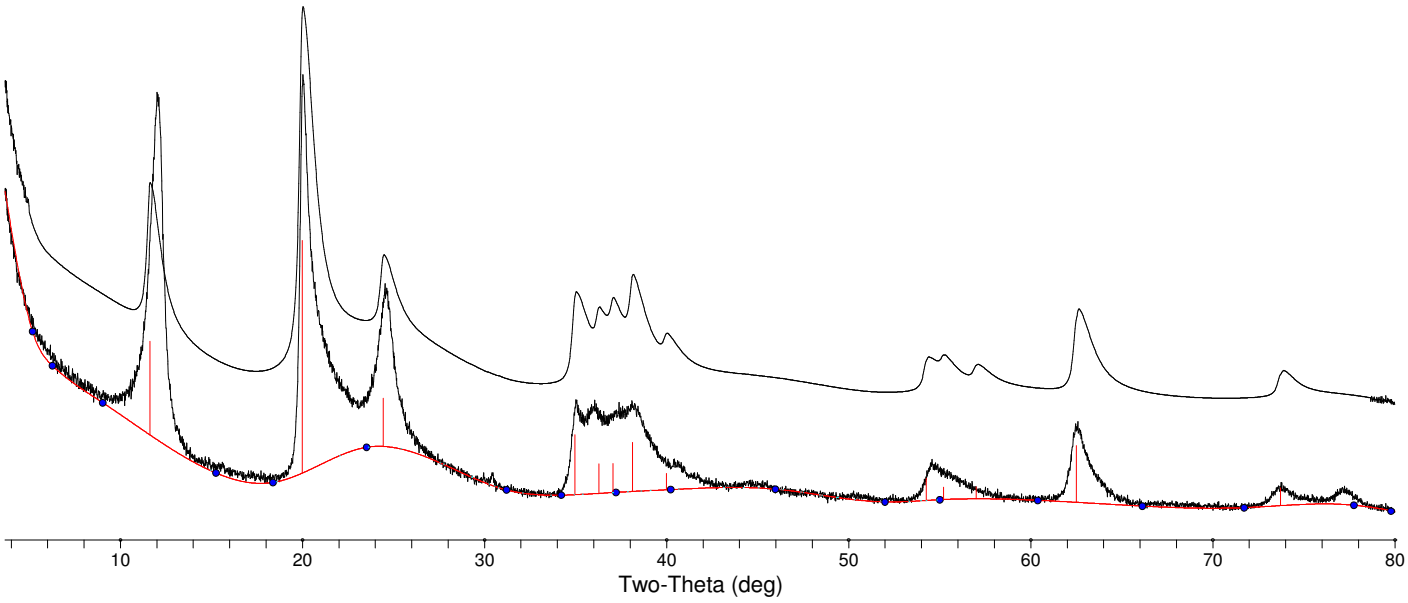
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (2)	Source	I/Ic	Wt%	#L	PC
Halloysite - $Al_2Si_2O_5(OH)_4$	PDF#00-060-1517	1.41(5%)	99.4 (7.2)	13	(020)=0.825
Nahcolite - $NaHCO_3$	PDF#00-015-0700	0.30(5%)	0.6 (0.0)	39	<None>

XRF(Wt%): Si=21.6%, Al=20.8%, Na=0.2%, O=55.8%, C=0.1%, H=1.6%

NOTE: Fitting Halted at Iteration 39(4): R=16.51% (E=2.99%, R/E=5.52, P=9, EPS=0.5)





Hematite coated quartzite BR93-25A

FILE: [Clipboard.mdi]
SCAN: 12.1/149.98/0.02/1(sec), Cu, I(p)=68230, 11/23/21 03:30p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\Clipboard.wpf] [Indi...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering
- ☑ Caglioti's FWHM Function

[Diffractometer LP] Two-Theta Range of Fit = 12.1 - 72.5(deg)

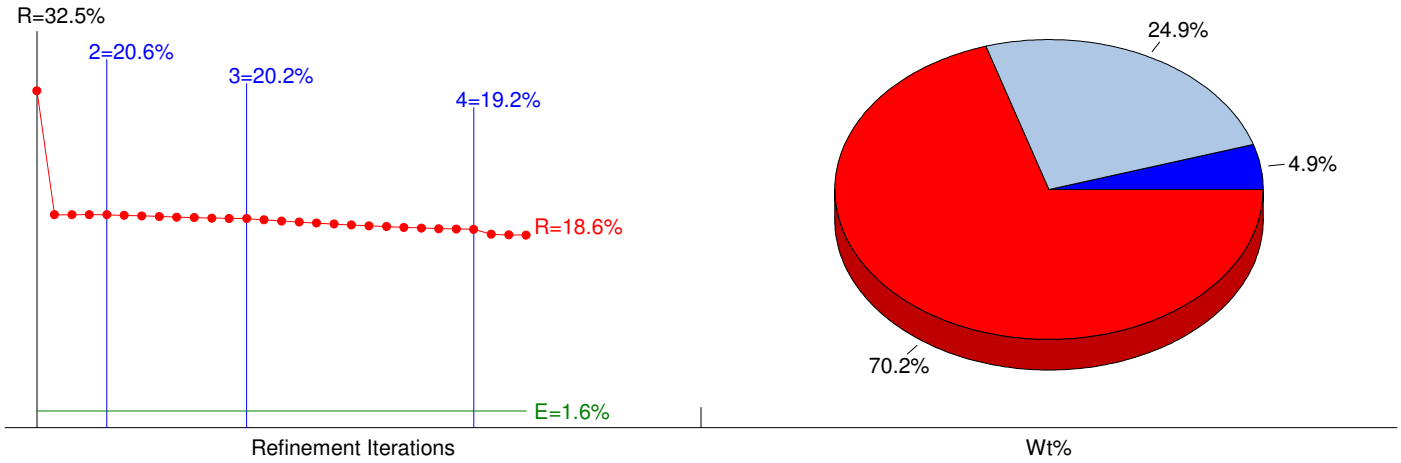
- ☑ Specimen Displacement - Cos(Theta) = -0.03926(0.010443)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

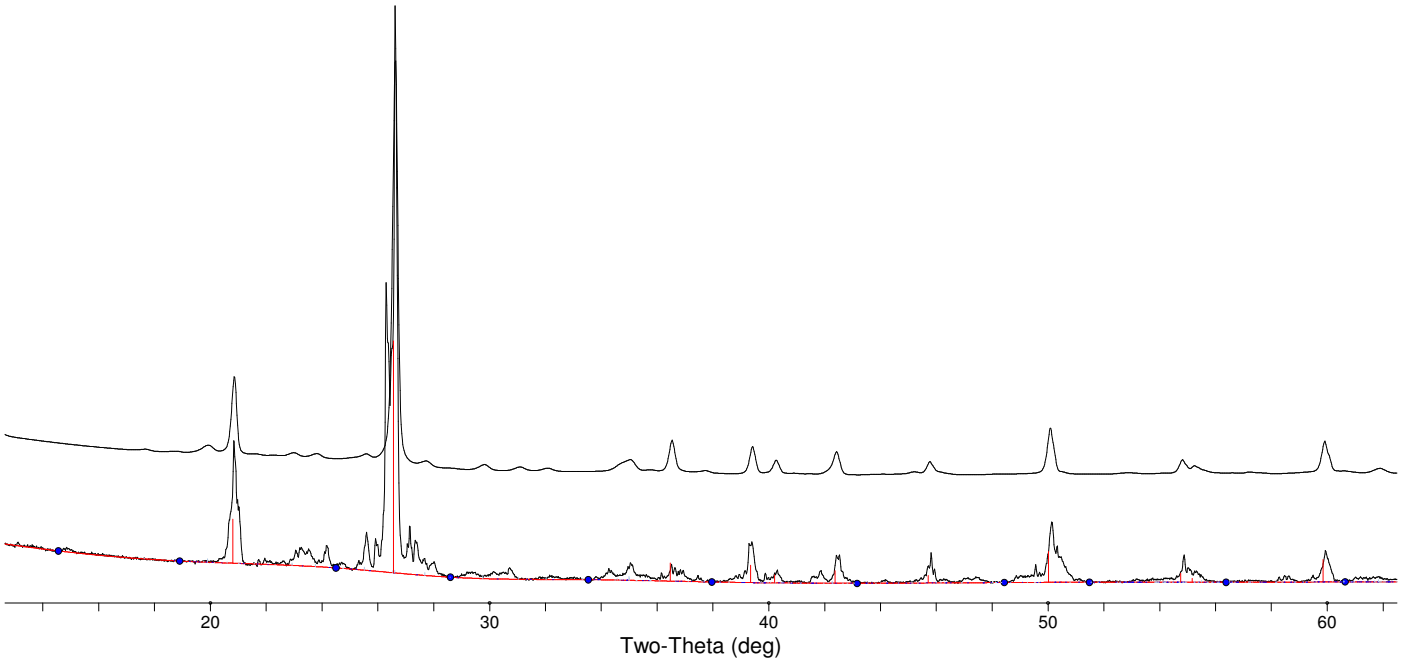
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (3)	Source	I/Ic	Wt%	#L
Clinochlore IIb - $Mg_{4.54}Al_{0.97}Fe_{0.46}Mn_{0.03}(Si_{2.85}Al_{1.15}O_{10})(OH)_8$	PDF#98-000-0165	0.80(0%)	4.9 (0.7)	297
Muscovite 2M - $KAl_2[Si_3Al]O_{10}(OH)_2$	PDF#98-000-0321	0.40(0%)	24.9 (1.6)	211
Quartz - SiO_2	PDF#98-000-0369	4.24(0%)	70.2 (2.0)	54

XRF(Wt%): Fe=0.2%, Mn=0.0%, K=2.5%, Si=38.8%, Al=5.6%, Mg=0.9%, O=51.9%, H=0.1%

NOTE: Fitting Halted at Iteration 29(4): R=18.6% (E=1.6%, R/E=11.63, P=21, EPS=0.5)





EMIT-Hematite_BR93-25B

FILE: [BR93-25B-Hematite.mdi] BR93-25B Hematite
SCAN: 12.22/62.08/0.02/1(sec), Cu, I(p)=62830, 11/23/21 11:04p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\BR93-25B-Hematit...

☑ K-alpha2 Peak Present
☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering

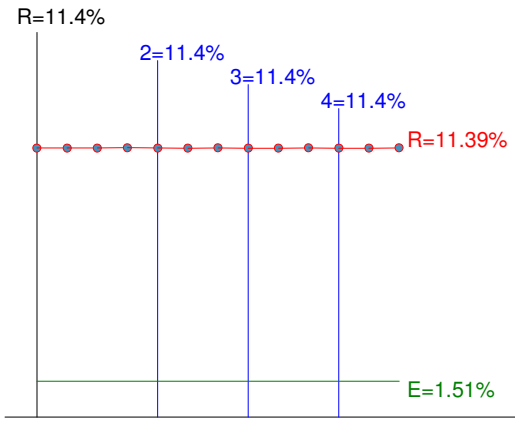
[Diffractometer LP] Two-Theta Range of Fit = 12.2 - 57.6(deg)
☑ Specimen Displacement - Cos(Theta) = 0.026852(0.011786)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

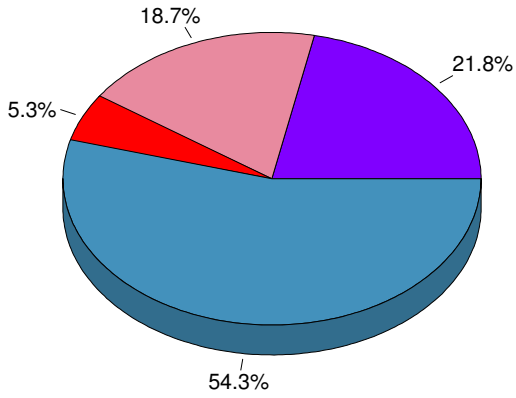
Phase ID (5)	Source	I/Ic	Wt%	#L
Albite - $Na(AlSi_3O_8)$	PDF#98-000-0041	0.64(0%)	21.8 (0.9)	163
Microcline - $K(AlSi_3O_8)$	PDF#98-000-0305	0.62(0%)	18.7 (1.0)	182
Hematite - Fe_2O_3	PDF#98-000-0240	3.13(0%)	5.3 (0.4)	10
Microcline - $KAlSi_3O_8$	PDF#00-019-0926	0.00(5%)	0.0 (0.0)	79
Quartz - SiO_2	PDF#00-046-1045	3.41(5%)	54.3 (3.3)	12

XRF(Wt%): Fe=3.7%, K=2.6%, Si=38.0%, Al=4.0%, Na=1.9%, O=49.7%

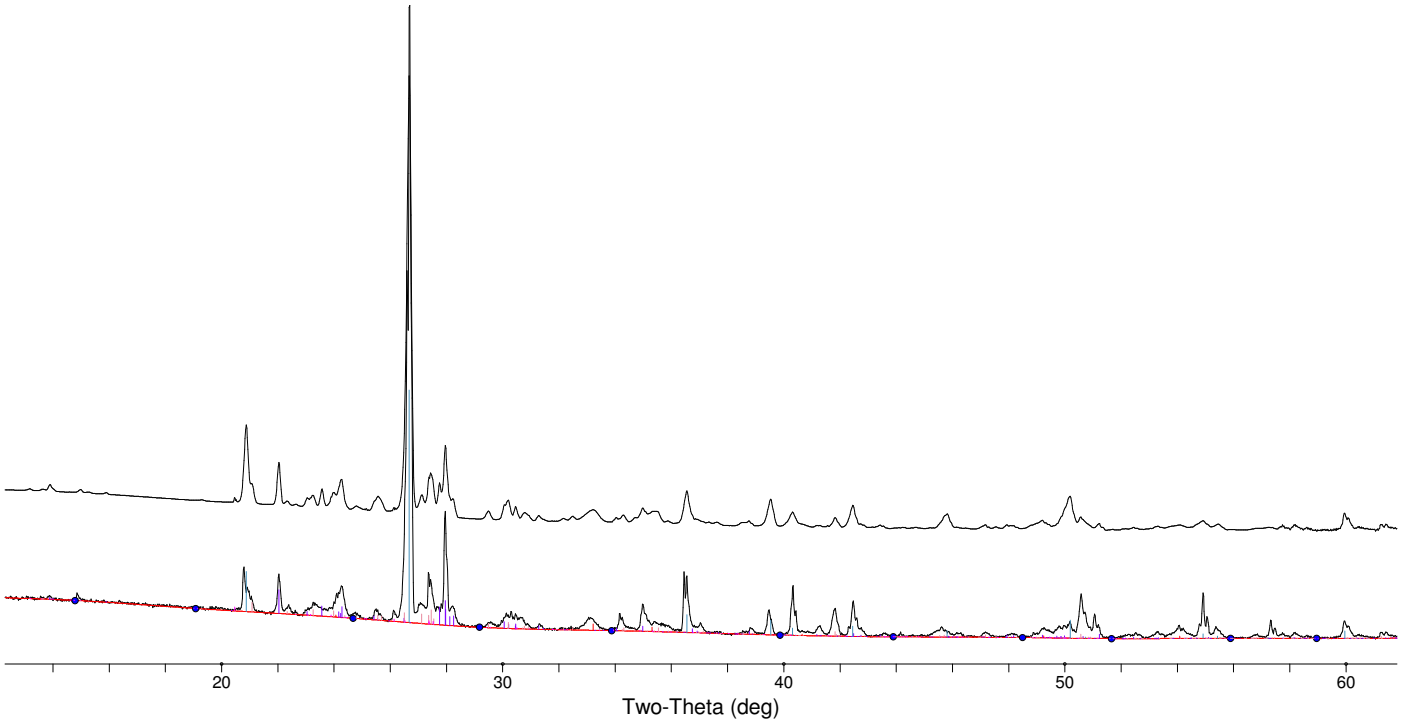
NOTE: Fitting Halted at Iteration 13(4): R=11.39% (E=1.51%, R/E=7.55, P=43, EPS=0.5)



Refinement Iterations



Wt%



EMIT-BR93-25C Hematite

FILE: [BR93-25C Hematite.mdi] BR93-25C Hematite
SCAN: 8.96/149.98/0.02/1(sec), Cu, I(p)=17376, 11/23/21 11:04p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\BR93-25C Hematit...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering
- ☑ Caglioti's FWHM Function

[Diffractometer LP] Two-Theta Range of Fit = 9.0 - 120.0(deg)

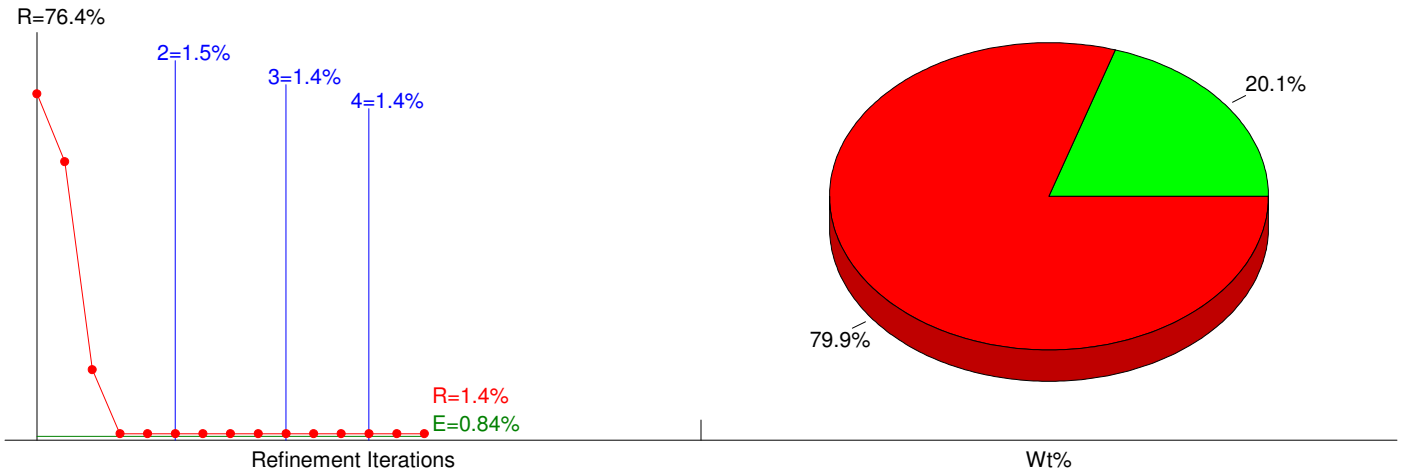
- ☑ Specimen Displacement - Cos(Theta) = -0.080745(0.033682)
- ☑ Axial Divergence - Cot(2Theta) = -0.081318(0.017866)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

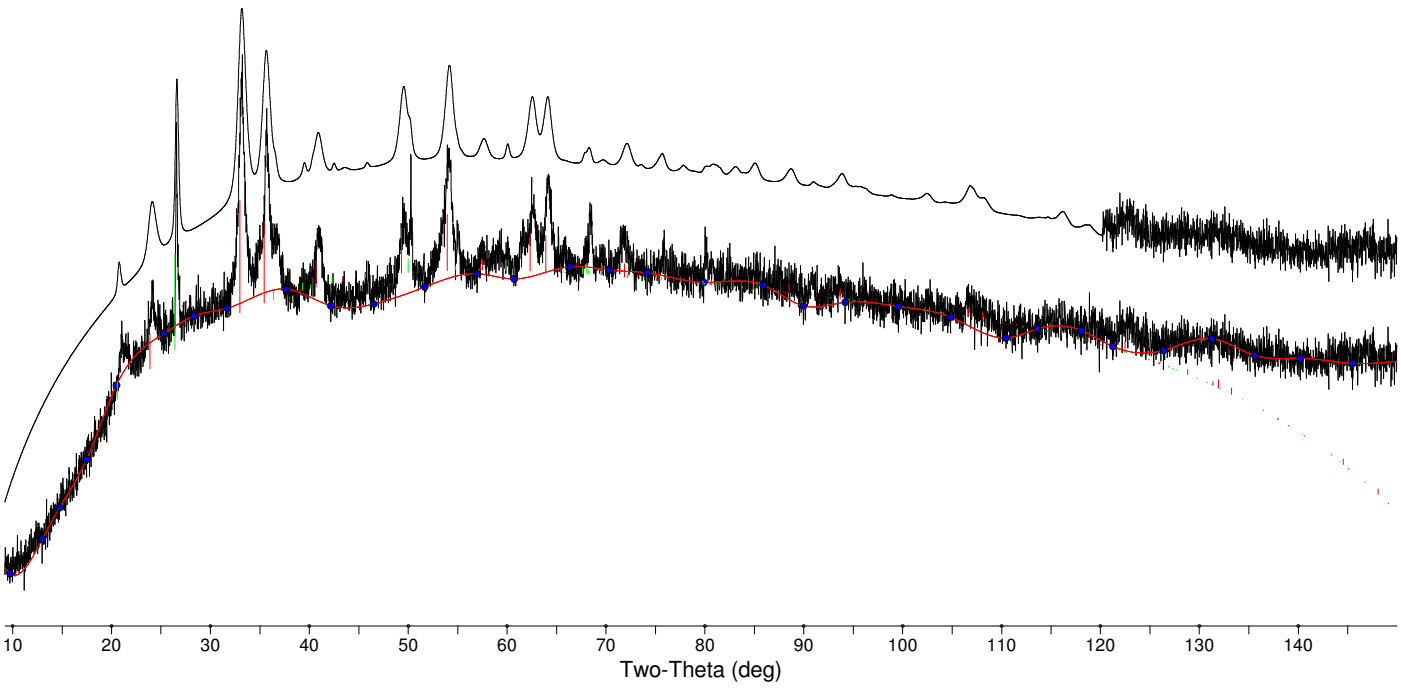
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Polynomial(4), Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (2)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#98-000-0369	4.30(0%)	20.1 (0.9)	154
Hematite - Fe_2O_3	PDF#98-000-0240	3.22(0%)	79.9 (2.5)	53

XRF(Wt%): Fe=55.9%, Si=9.4%, O=34.7%

NOTE: Fitting Halted at Iteration 15(4): R=1.4% (E=0.84%, R/E=1.68, P=18, EPS=0.5)





EMIT-Hematite BR93-34C

FILE: [BR93-34C Hematite.mdi]
SCAN: 9.32/149.98/0.02/1(sec), Cu, I(p)=15918, 11/23/21 10:13p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\BR93-34C Hematit...

- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering
- ☑ Caglioti's FWHM Function

[Diffractometer LP] Two-Theta Range of Fit = 9.3 - 120.0(deg)

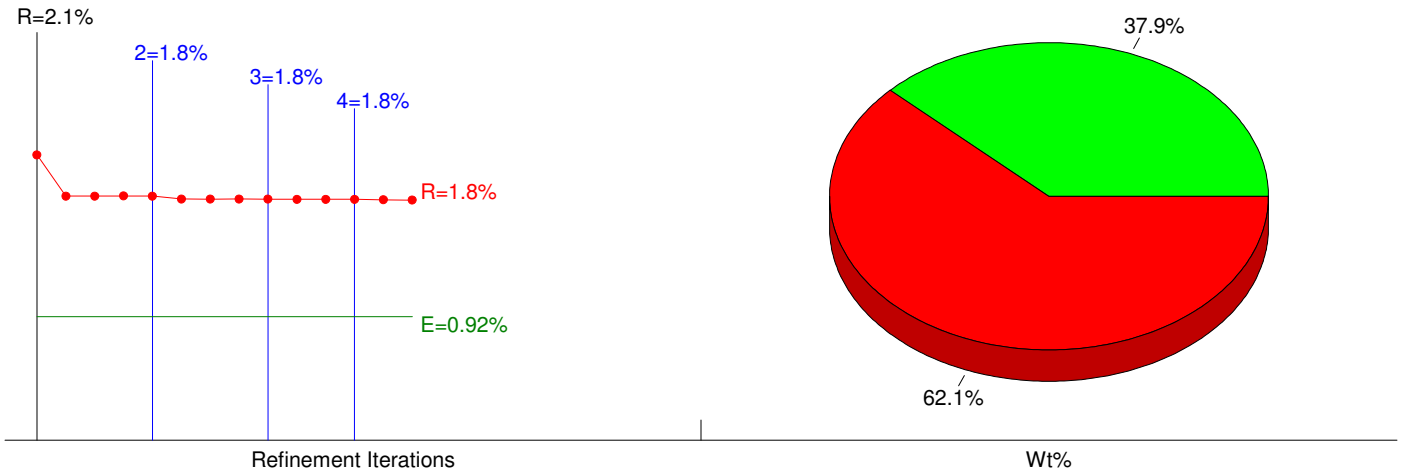
- ☑ Zero Offset of Goniometer - 2Theta = 0.247296(0.084486)
- ☑ Specimen Displacement - Cos(Theta) = -0.376927(0.088123)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

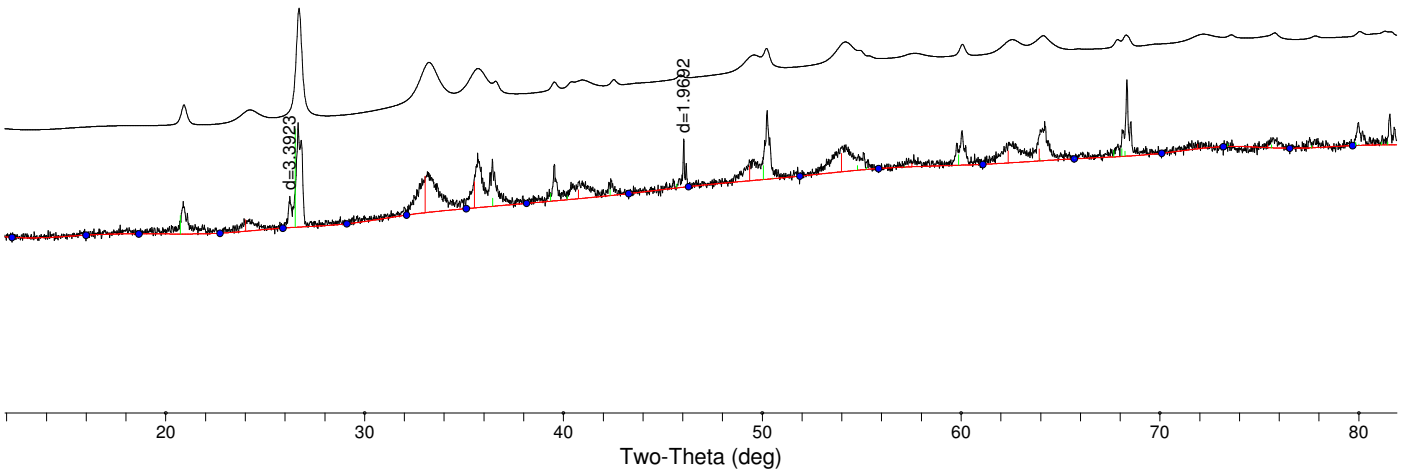
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

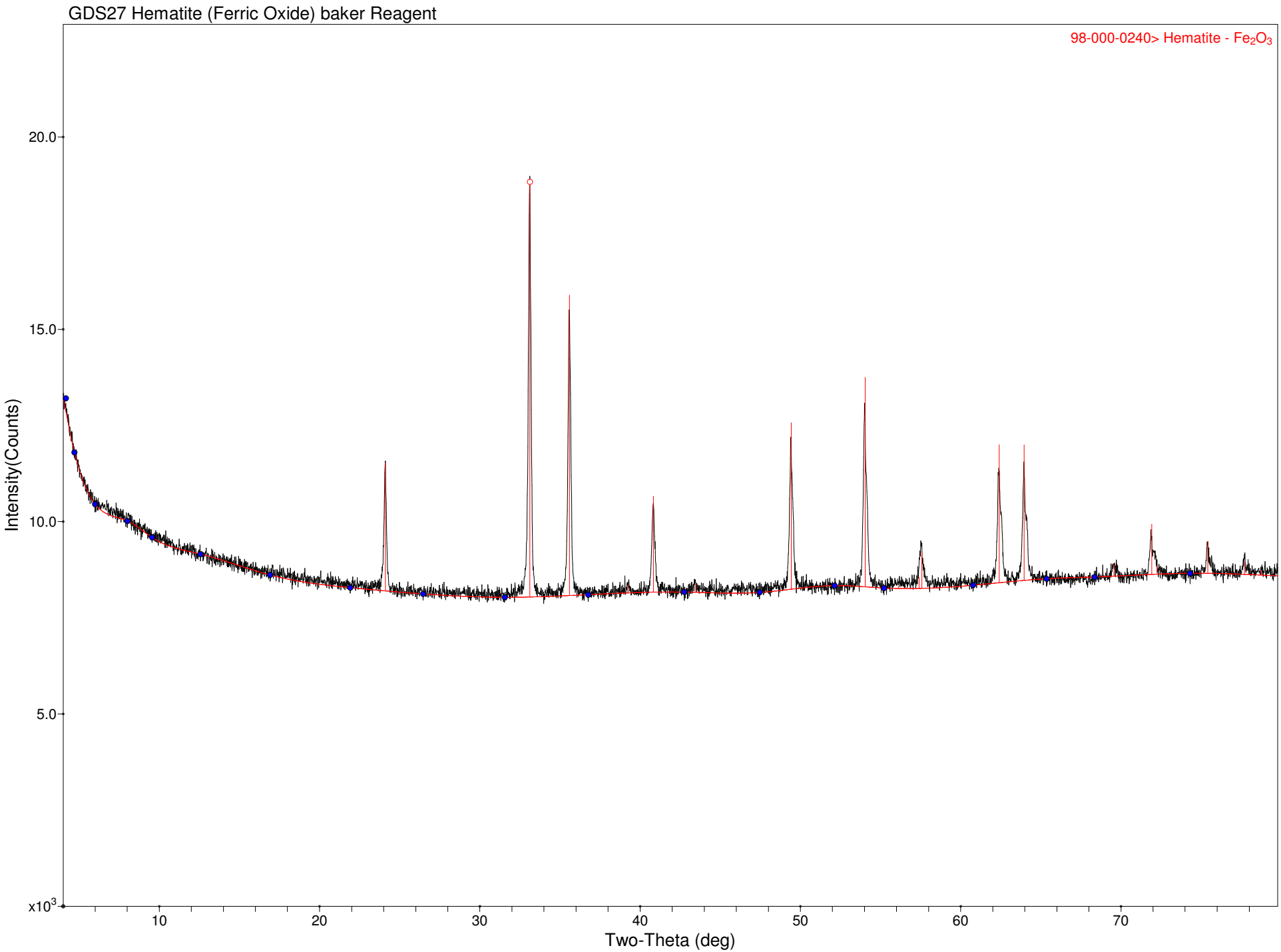
Phase ID (2)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#98-000-0369	4.26(0%)	37.9 (0.7)	154
Hematite - Fe_2O_3	PDF#98-000-0240	3.20(0%)	62.1 (1.0)	53

XRF(Wt%): Fe=43.5%, Si=17.7%, O=38.8%

NOTE: Fitting Halted at Iteration 14(4): R=1.8% (E=0.92%, R/E=1.94, P=12, EPS=0.5)






GDS27 Hematite (Ferric Oxide) baker Reagent
98-000-0240> Hematite - Fe_2O_3
20.0
15.0
10.0
5.0
x10^3
Intensity(Counts)
10
20
30
40
50
60
70
Two-Theta (deg)

EMIT-WS161.1 Hematite, Cumberland, England

FILE: [MRP-19496_C-522668_EMIT_WS161-1.xrdml] WS161.1 Hematite, Cumberland, England
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=10150, 08/26/21 03:20a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108008_WBSSS-6369_Swayze_EMIT-Group-3\MRP-19496_C-5...

☑ K-alpha2 Peak Present
☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering

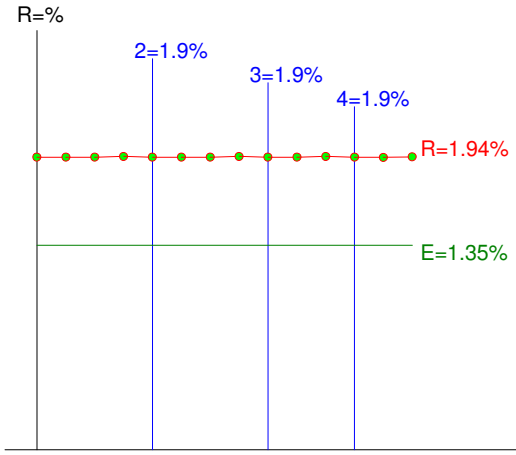
[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)
☑ Specimen Displacement - Cos(Theta) = -0.043978(0.004644)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

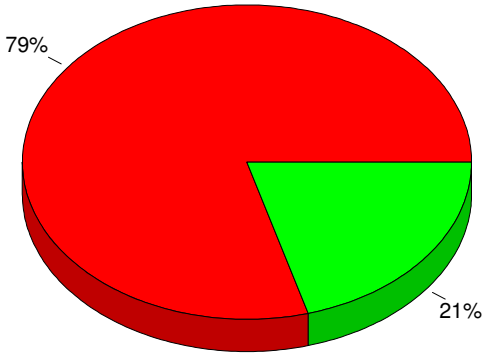
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

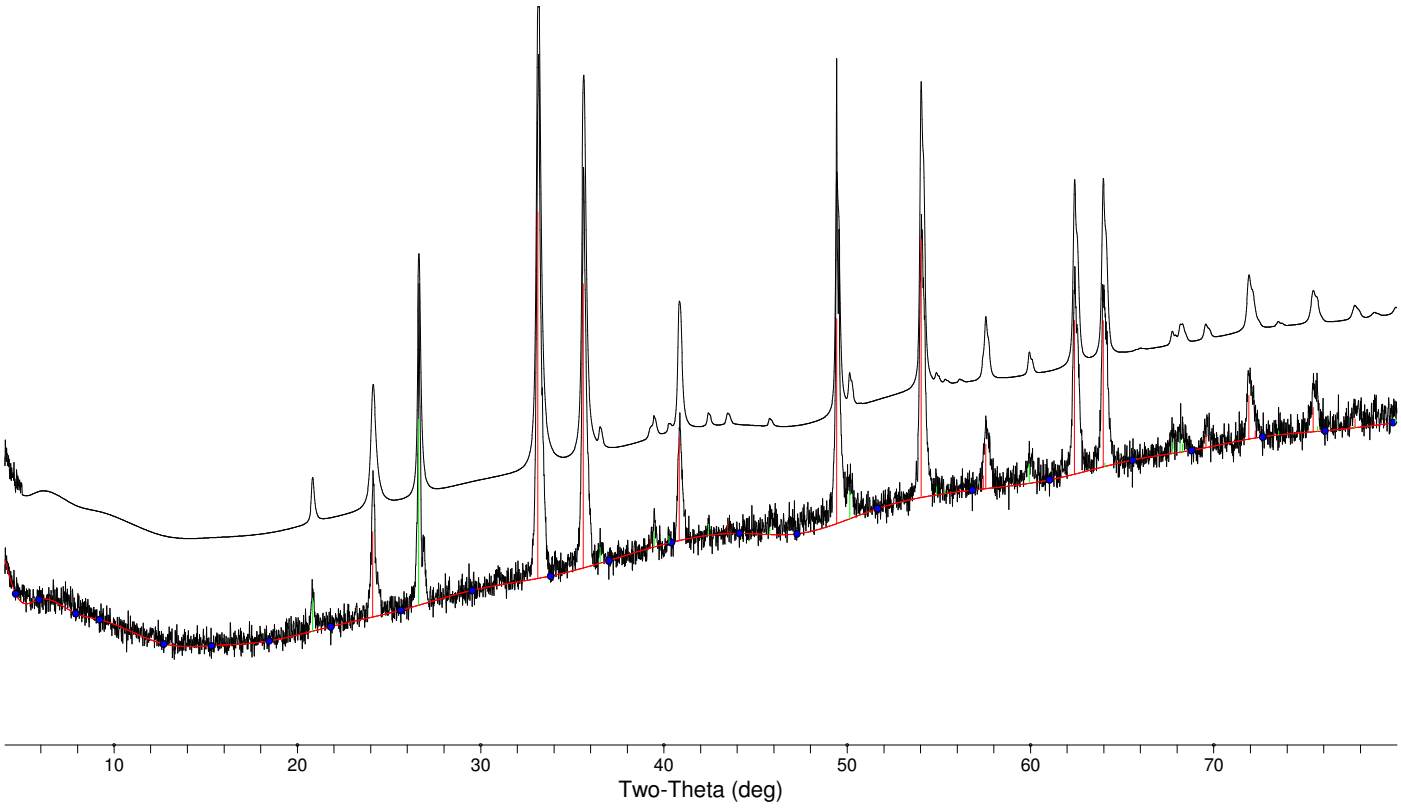
Phase ID (2)	Source	I/Ic	Wt%	#L
Hematite - Fe_2O_3	PDF#98-000-0240	3.18(0%)	79 (1)	23
Quartz - SiO_2	PDF#98-000-0369	4.24(0%)	21 (0)	68

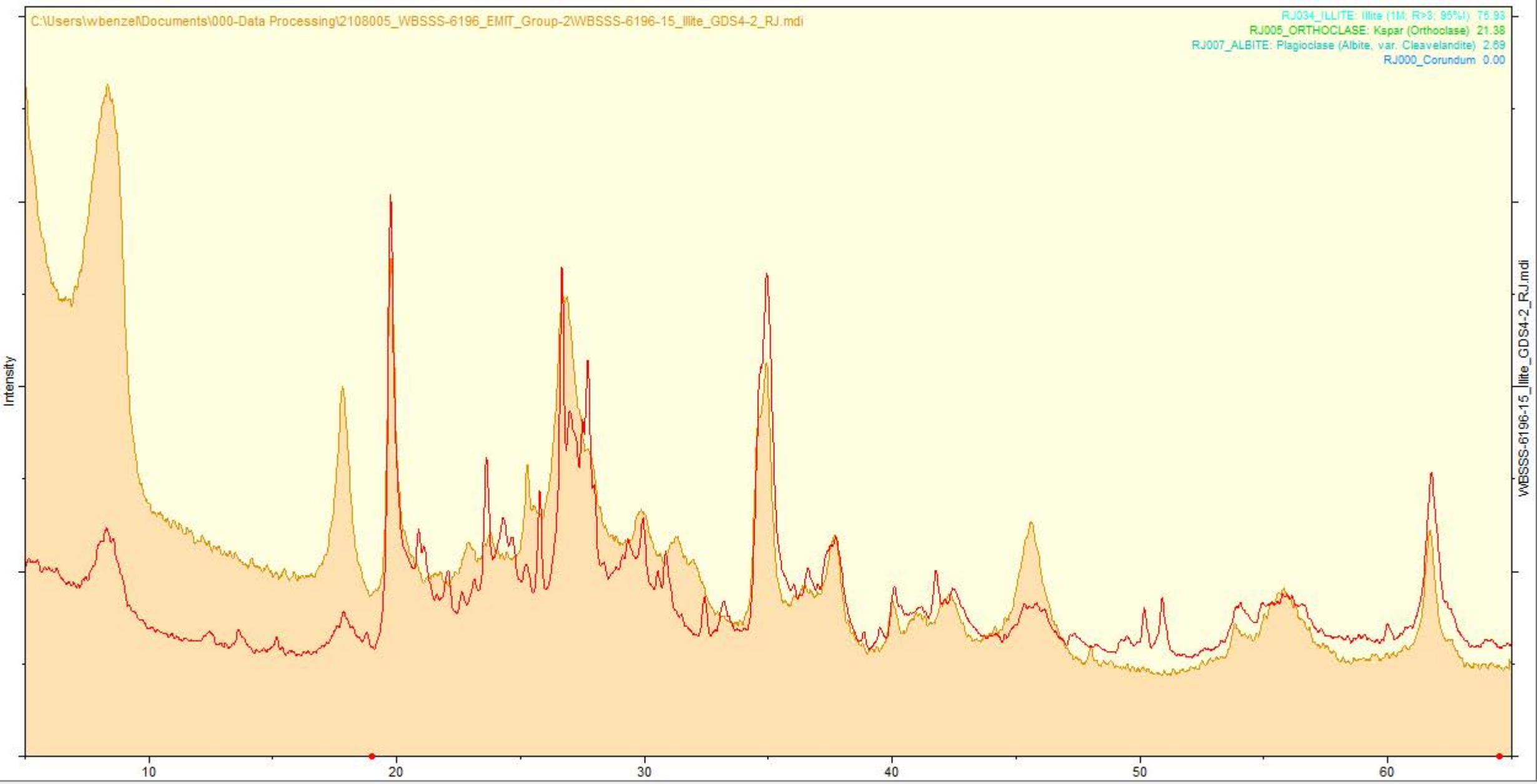
XRF(Wt%): Fe=56%, Si=10%, O=35%

NOTE: Fitting Halted at Iteration 14(4): R=1.94% (E=1.35%, R/E=1.43, P=18, EPS=0.5)









(3) MIF [5-65] Al2O3 | 0 | 0.5 | 100 | 12 LSR cycles, Rp=15.86%, d2T=-0.02, Rwp=19.39%

#	Description	Scale	Best w[%]	d2Th	MIF	Rank
☑ 1	RJ000_Corundum	0.0000	0.00	0.00	1	0.27
☑ 34	**RJ034_ILLITE: Illite (1M; R>3; 95%I)**	23.6568	75.93	-0.020	1.565	0.54
☑ 6	**RJ005_ORTHOCLASE: Kspar (Orthoclase)**	4.5057	21.38	-0.020	1.683	0.18
☑ 8	**RJ007_ALBITE: Plagioclase (Albite, var. Cleavel...**	0.4675	2.69	-0.020	1.479	0.05

EMIT-Illite, IMt-1 <2u

FILE: [WBSSS-6196-16_1Mt-1_rep.xrdml] Illite, IMt-1 <2u
SCAN: 2.0084/79.9999/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=39776, 08/23/21 10:12a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108005_WBSSS-6196_EMIT_Group-2\WBSSS-6196-16_1Mt-1_...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 67.7(deg)

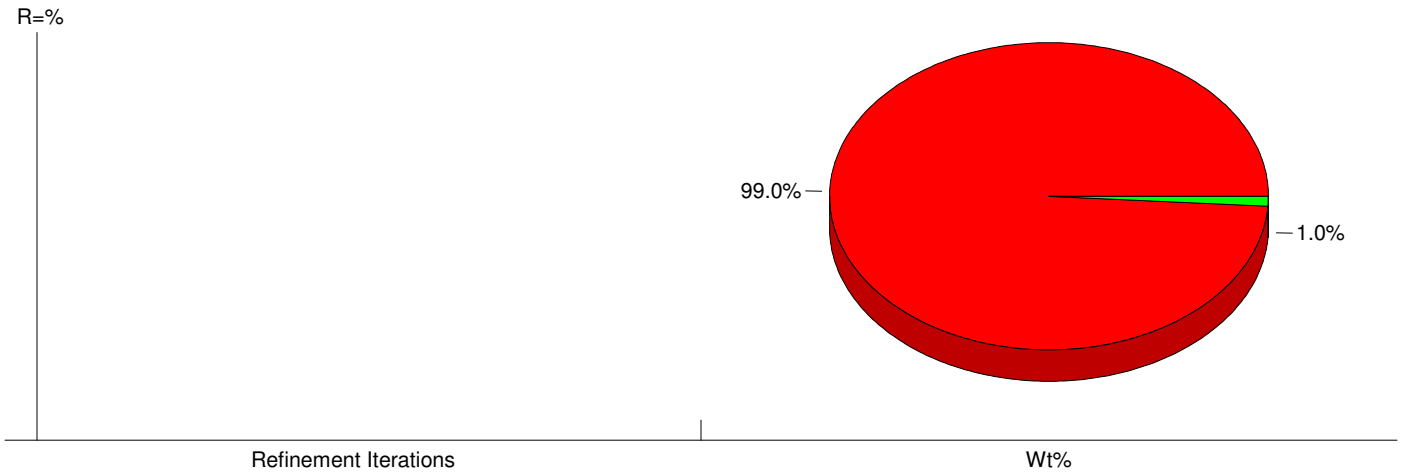
- ☑ Zero Offset of Goniometer - 2Theta = -0.759434(0.178214)
- ☑ Specimen Displacement - Cos(Theta) = 0.758442(0.18513)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

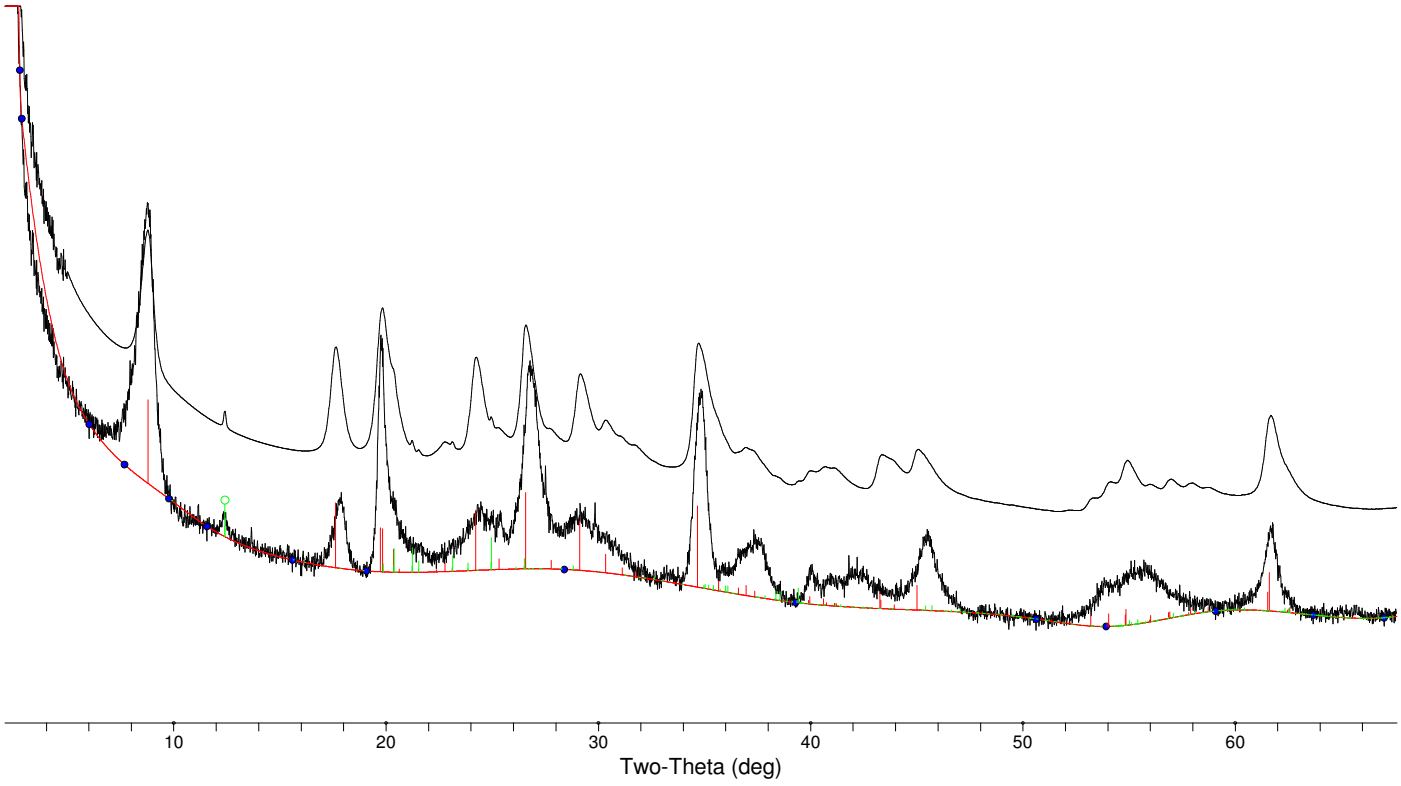
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (2)	Source	I/Ic	Wt%	#L	PC
Illite - $KAl_2(Si_3Al)O_{10}(OH)_2$	PDF#00-043-0685	0.36(5%)	99.0 (7.4)	50	SHF(6,3)
Kaolinite - $Al_4(OH)_8(Si_4O_{10})$	PDF#98-000-0261	0.86(0%)	1.0 (0.1)	511	<None>

XRF(Wt%): K=9.7%, Si=21.2%, Al=20.3%, O=48.3%, H=0.5%

NOTE: Fitting Halted at Iteration 0(1): R=10.92% (E=2.85%, R/E=3.83, P=13, EPS=0.5)





EMIT-GDS76 Hematite-2wt% + Qtz

FILE: [Wbsss-6196-07_EMIT_Intimate-mix.xrdml] GDS76 Hematite-2wt% + Qtz
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=136767, 08/24/21 03:00p
PROC: [WPF Control File]

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)

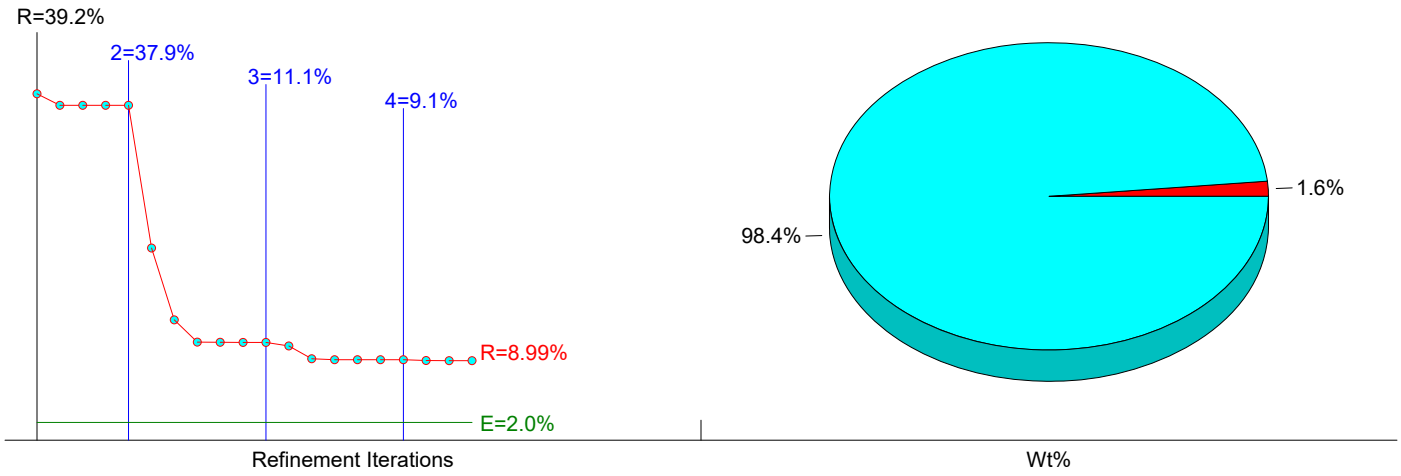
- ☑ Zero Offset of Goniometer - 2Theta = -0.111361(0.008494)
- ☑ Specimen Displacement - Cos(Theta) = 0.067081(0.009019)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

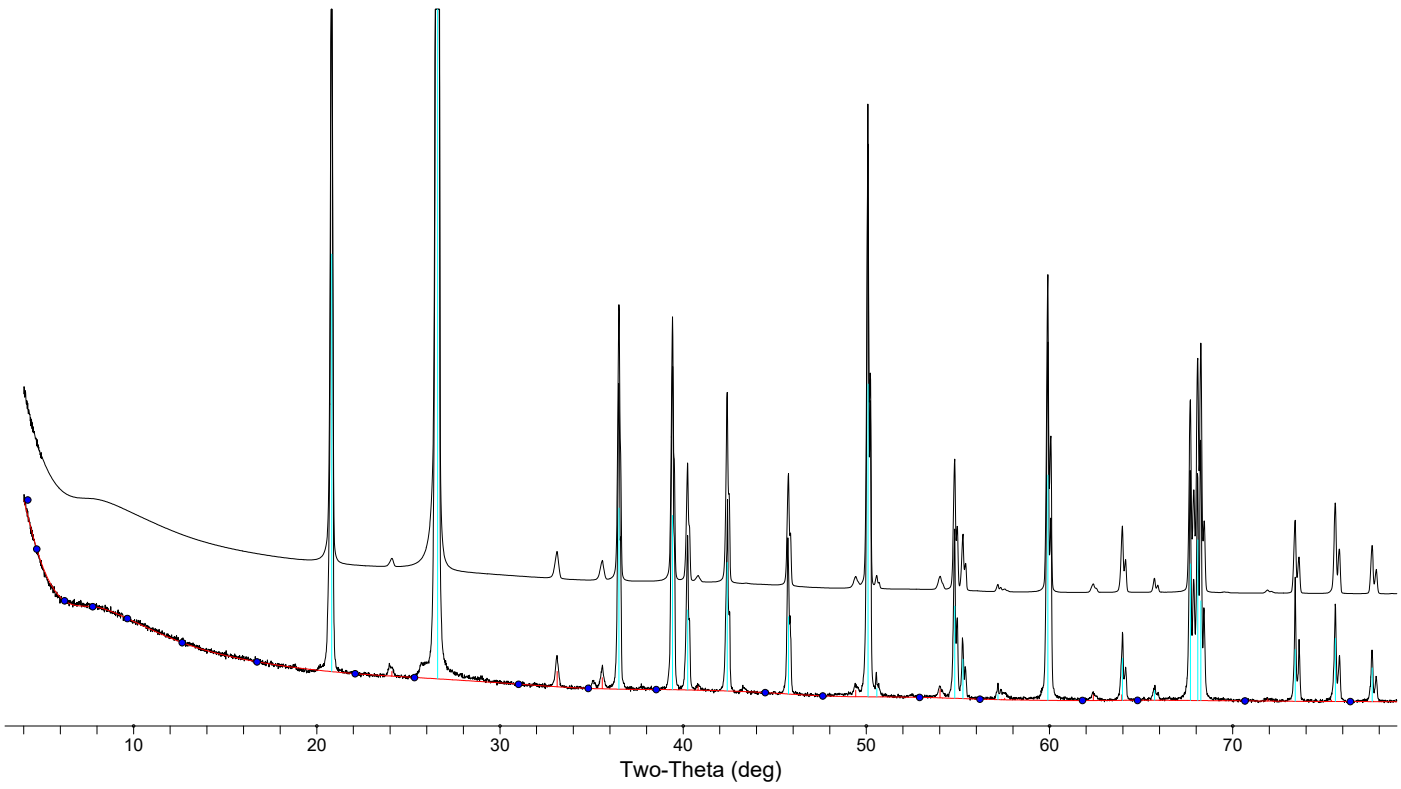
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (2)	Source	I/Ic	Wt%	#L
Hematite - Fe_2O_3	PDF#98-000-0240	3.18(0%)	1.6 (0.1)	23
Quartz - SiO_2	PDF#98-000-0369	4.24(0%)	98.4 (0.4)	70

XRF(Wt%): Fe=1.1%, Si=46.0%, O=52.9%

NOTE: Fitting Halted at Iteration 20(4): R=8.99% (E=2.0%, R/E=4.5, P=13, EPS=0.5)





EMIT-CM9 Kaolinite,

FILE: [MRP-19177_C-522589_Kaolinite_CM9.xrdml] CM9 Kaolinite,
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=61832, 08/25/21 04:13a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2105001 MRP-19177_Swayze_EMIT_Group-1\MRP-19177_C-522...

☑ K-alpha2 Peak Present
☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering

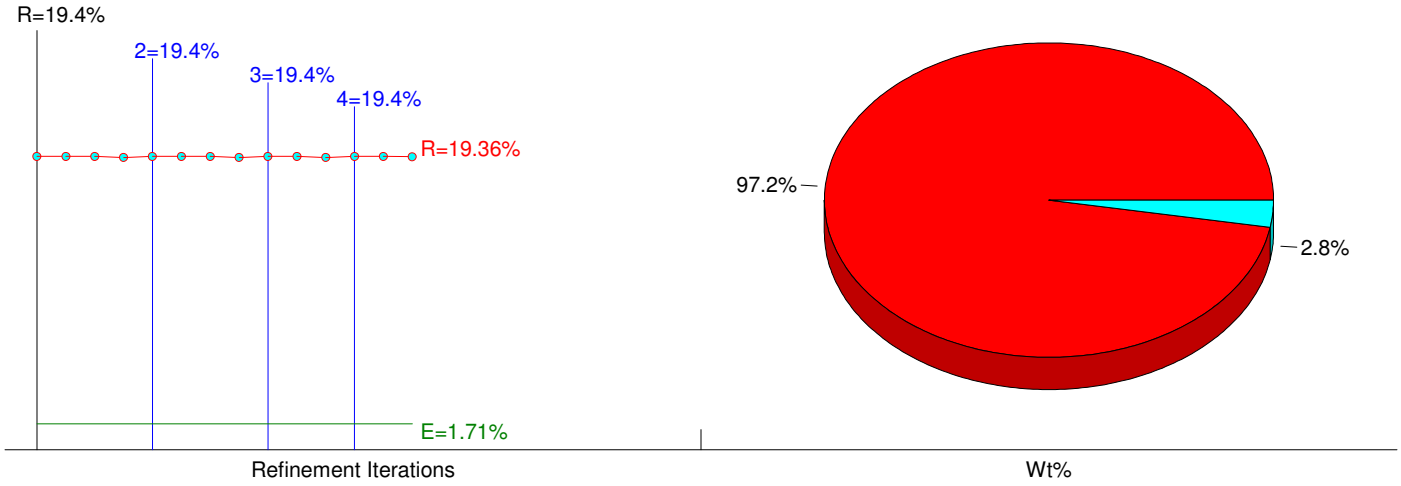
[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 74.6(deg)
☑ Specimen Displacement - Cos(Theta) = -0.007809(0.003166)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

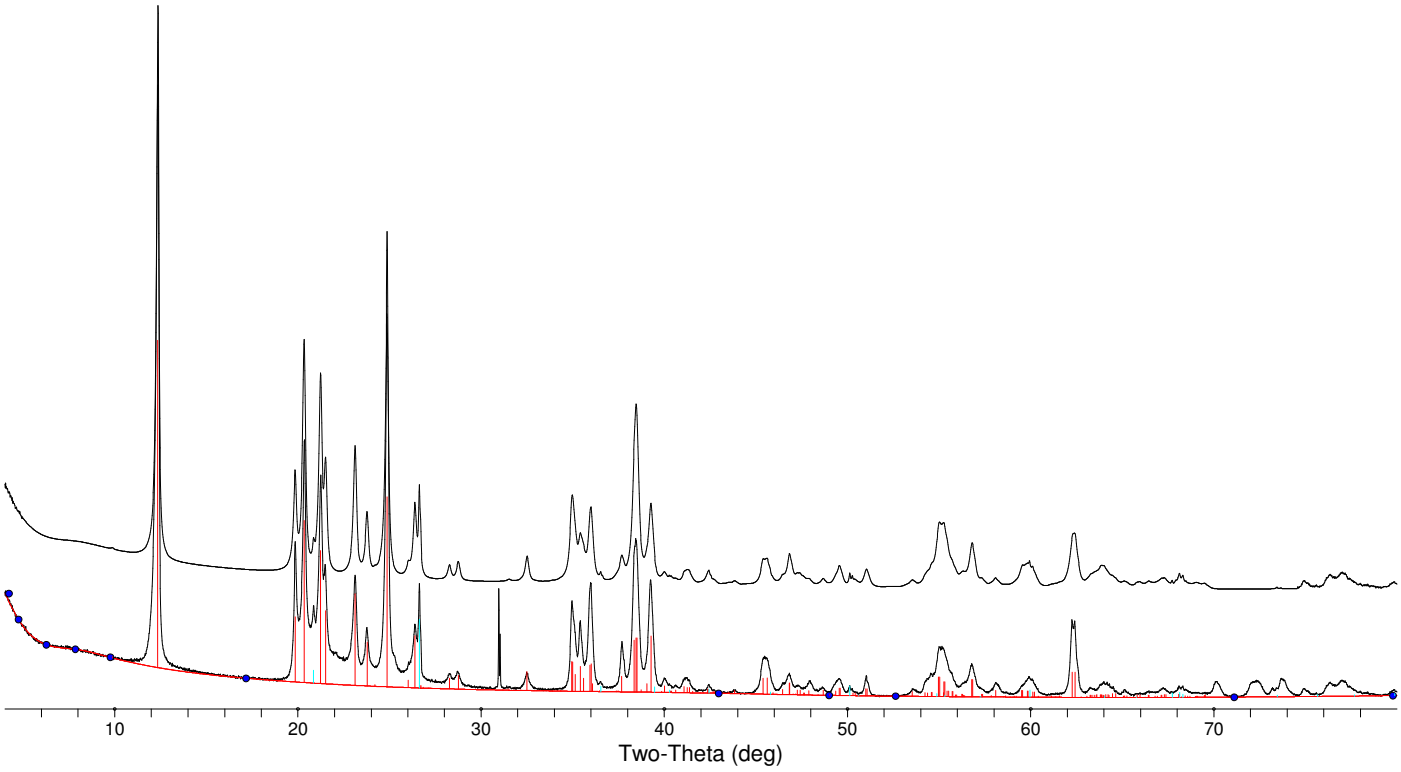
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (2)	Source	I/Ic	Wt%	#L
Kaolinite - $Al_2(Si_2O_5)(OH)_4$	PDF#01-080-0886	1.10(5%)	97.2 (6.8)	199
Quartz - SiO_2	PDF#98-000-0369	4.22(0%)	2.8 (0.2)	58

XRF(Wt%): Si=22.4%, Al=20.3%, O=55.7%, H=1.5%

NOTE: Fitting Halted at Iteration 14(4): R=19.36% (E=1.71%, R/E=11.32, P=18, EPS=0.5)





KGa-1-Kaolinite_Washington Co., Georgia

FILE: [MRP-19177_C-522590_Kaolinite_KGa-1.xrdml] KGa-1 Kaolinite Washington Co., Georgia
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=74874, 08/25/21 05:30a
PROC: [WPF Control File]

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)

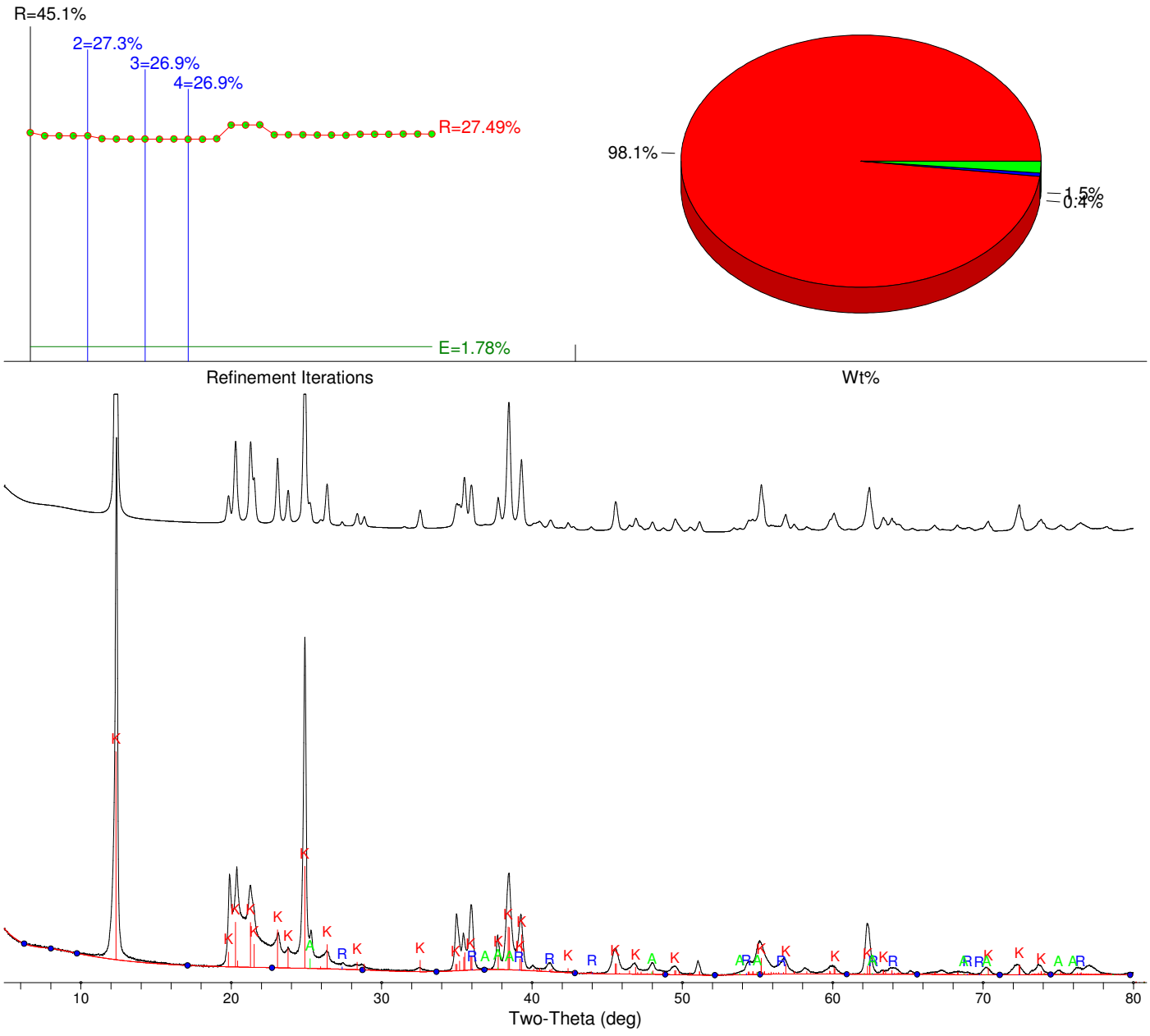
- ☑ Specimen Displacement - Cos(Theta) = -0.068314(0.00338)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

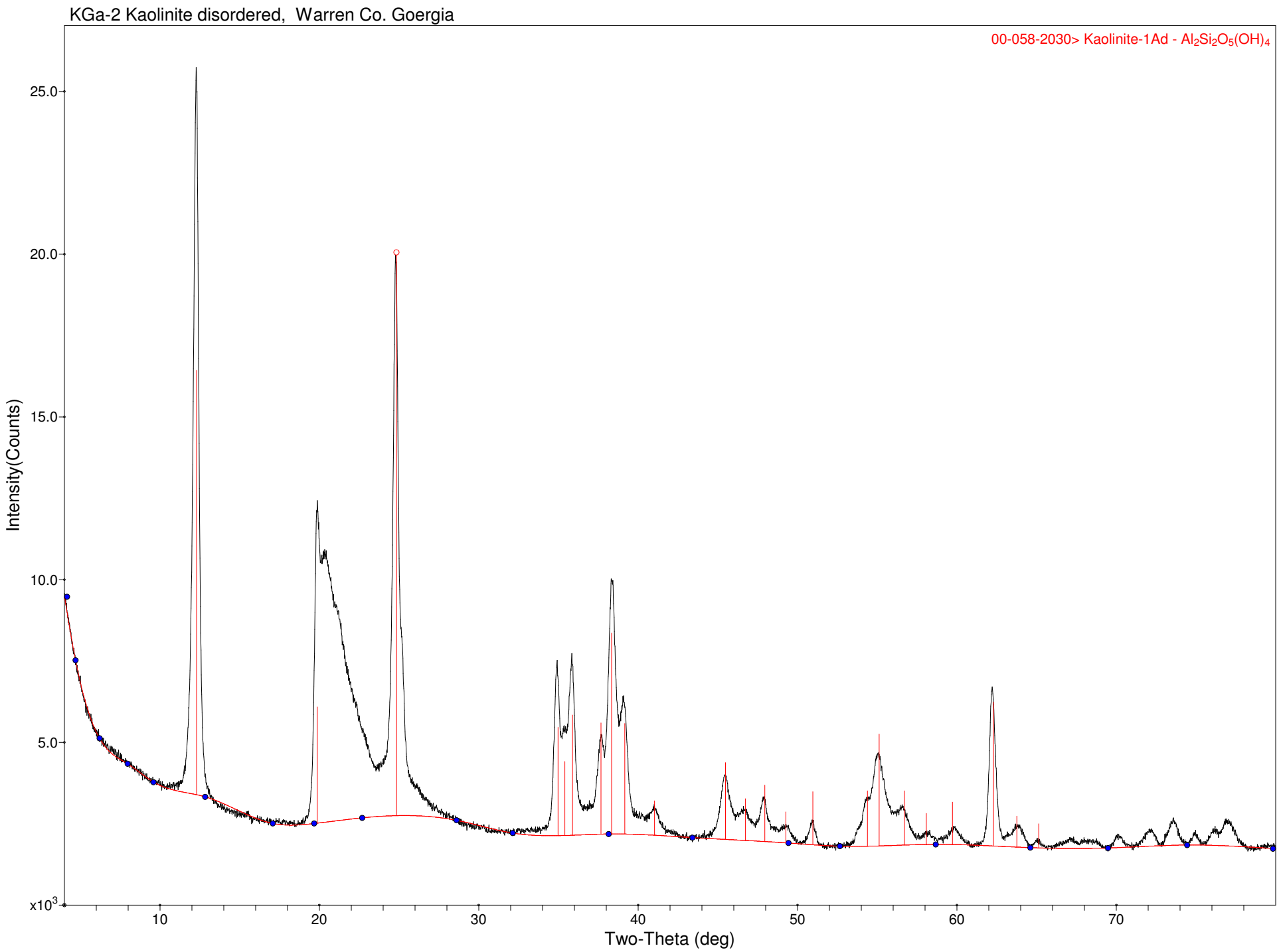
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (3)	Source	I/Ic	Wt%	#L	PC
Kaolinite - $Al_2Si_2O_5(OH)_4$	PDF#01-075-1593	1.20(5%)	98.1 (7.0)	165	(001)=0.900
Rutile - TiO_2	PDF#98-000-0375	3.41(0%)	0.4 (0.0)	16	<None>
Anatase - TiO_2	PDF#98-000-0081	5.13(0%)	1.5 (0.1)	32	<None>

XRF(Wt%): Ti=1.2%, Si=21.3%, Al=20.5%, O=55.5%, H=1.5%

NOTE: Fitting Halted at Iteration 29(4): R=27.49% (E=1.78%, R/E=15.45, P=8, EPS=0.5)




KGa-2 Kaolinite disordered, Warren Co. Goergia
00-058-2030> Kaolinite-1Ad - $Al_2Si_2O_5(OH)_4$
Intensity(Counts)
25.0
20.0
15.0
10.0
5.0
x10^3
10
20
30
40
50
60
70
Two-Theta (deg)

EMIT-CU93-5C Kaolinite + Muscovite Intimate Mixture

FILE: [MRP-19498_C-522679_EMIT_CU93-5C.xrdml] CU93-5C Kaolinite + Muscovite Intimate Mixture
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=128535, 12/17/21 09:51a
PROC: [WPF Control File]

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)

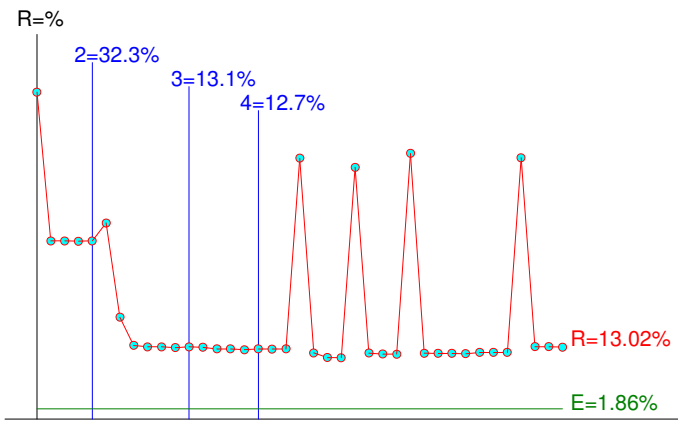
- ☑ Zero Offset of Goniometer - 2Theta = -0.059128(0.011848)
- ☑ Specimen Displacement - Cos(Theta) = 0.13444(0.012659)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

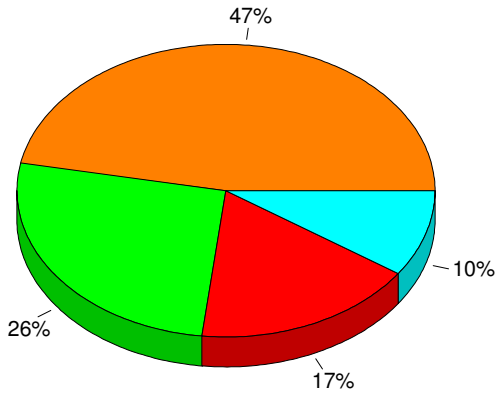
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

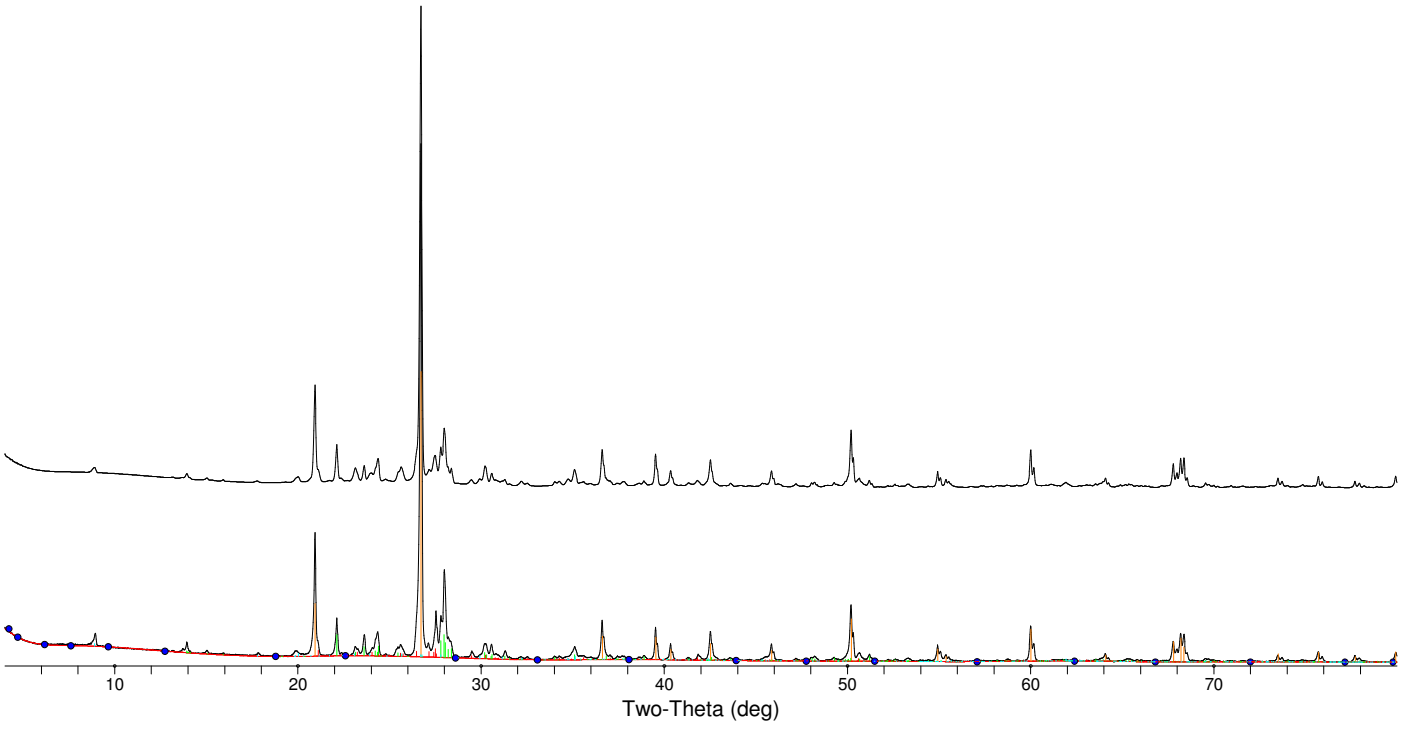
Phase ID (4)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#98-000-0369	4.20(0%)	47 (0)	68
Albite - $Na(AlSi_3O_8)$	PDF#98-000-0041	0.64(0%)	26 (0)	383
Microcline - $K(AlSi_3O_8)$	PDF#98-000-0305	0.62(0%)	17 (0)	423
Muscovite 2M - $KAl_2[Si_3Al]O_{10}(OH)_2$	PDF#98-000-0321	0.40(0%)	10 (0)	293

XRF(Wt%): K=3%, Si=38%, Al=6%, Na=2%, O=50%

NOTE: Fitting Halted at Iteration 39(4): R=13.02% (E=1.86%, R/E=7.0, P=11, EPS=0.5)







EMIT-GDS80 Lepidocrocite Synthetic

FILE: [Wbsss-6196-09_EMIT_Lepidocrosite.xrdml] GDS80 Lepidolite Synthetic
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=14982, 08/24/21 07:26p
PROC: [WPF Control File]

☑ K-alpha2 Peak Present
☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering

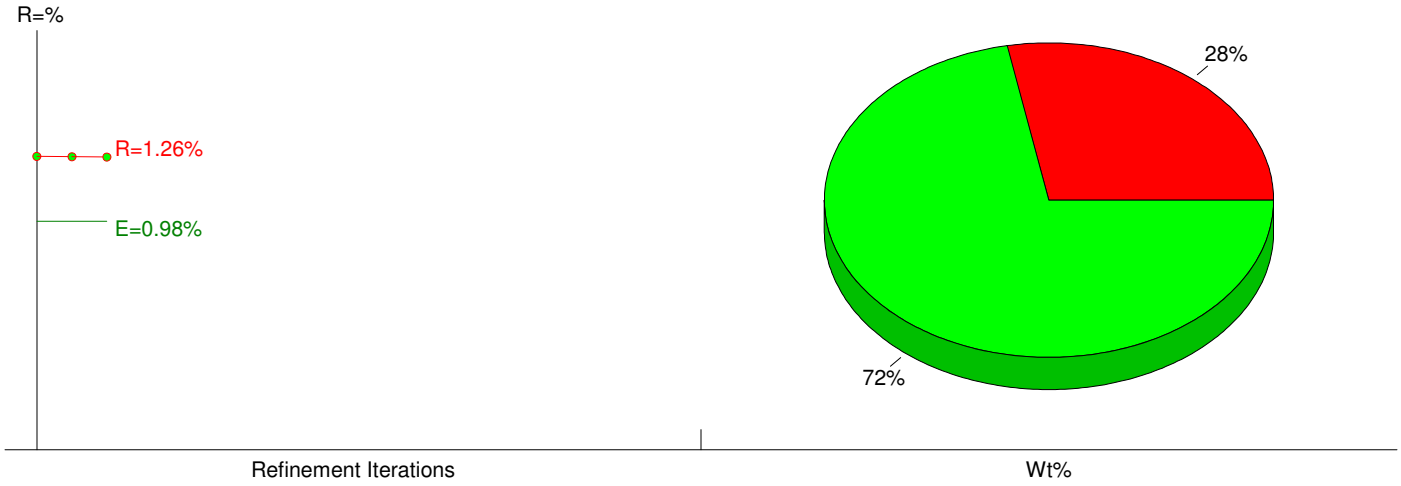
[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)
☑ Specimen Displacement - Cos(Theta) = -0.034613(0.01356)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

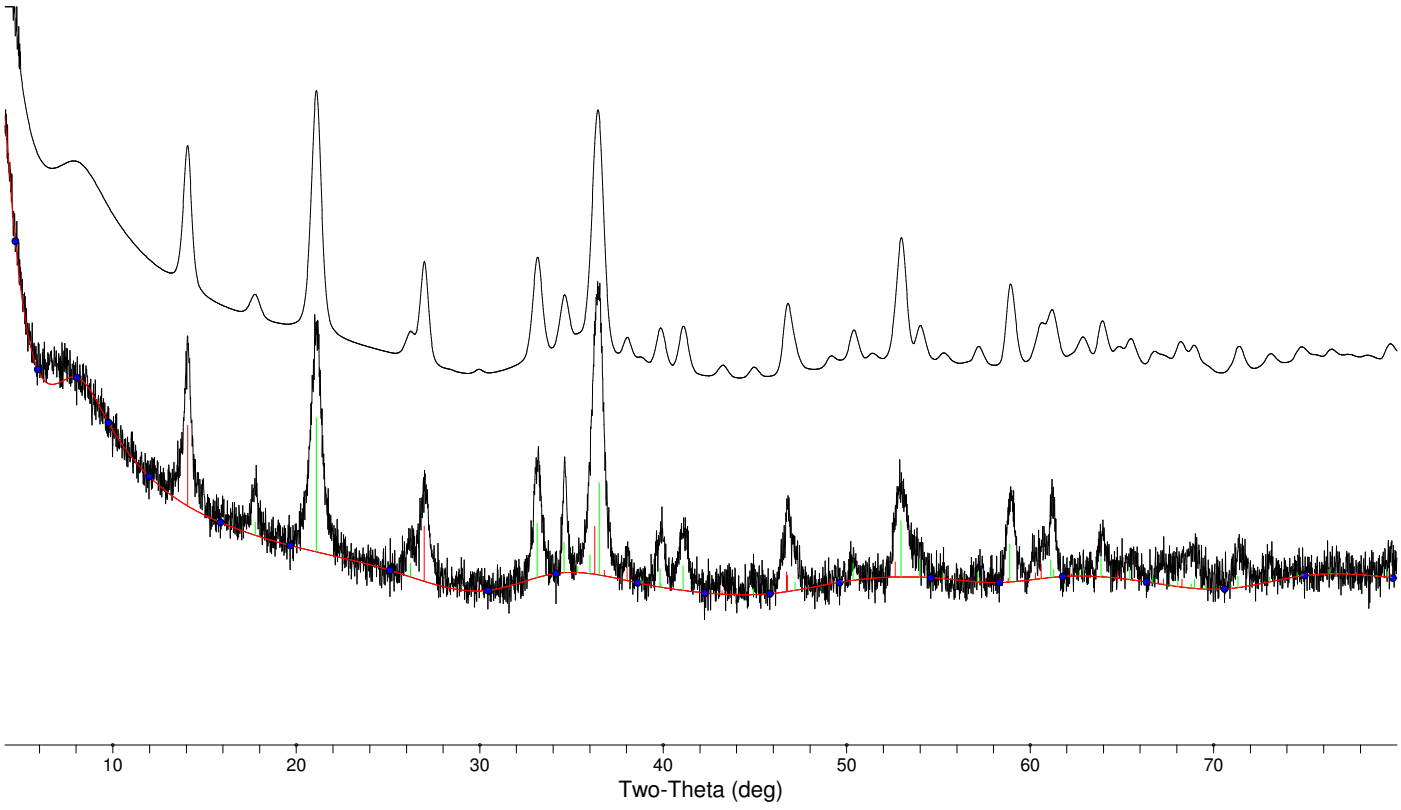
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (2)	Source	I/Ic	Wt%	#L	PS*	LAC
Lepidocrocite - FeO(OH)	PDF#04-010-4300	3.79(0%)	28 (1)	36	1.0	782.1
Goethite - FeO(OH)	PDF#04-015-2900	2.97(0%)	72 (1)	57	1.0	834.5

XRF(Wt%): Fe=63%, O=36%, H=0%

NOTE: Fitting Halted at Iteration 3(4): R=1.26% (E=0.98%, R/E=1.28, P=20, EPS=0.5), *Particle Size for Brindley Correction





GDS81 Synthetic MaEMIT-ghemite

FILE: [MRP-19496_C-522669_EMIT_GDS81.xrdml] GDS81 Synthetic Maghemite
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=13128, 08/26/21 04:38a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108008_WBSSS-6369_Swayze_EMIT-Group-3\MRP-19496_C-5...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 15.0 - 70.0(deg)

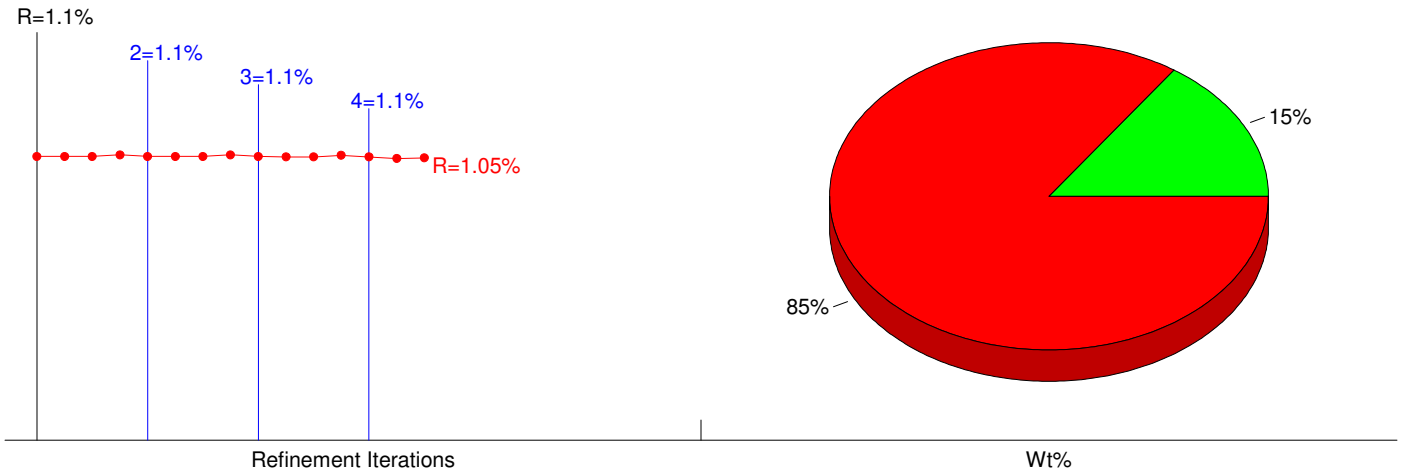
- ☑ Zero Offset of Goniometer - 2Theta = 0.861366(1.01214)
- ☑ Specimen Displacement - Cos(Theta) = -0.865784(0.970833)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

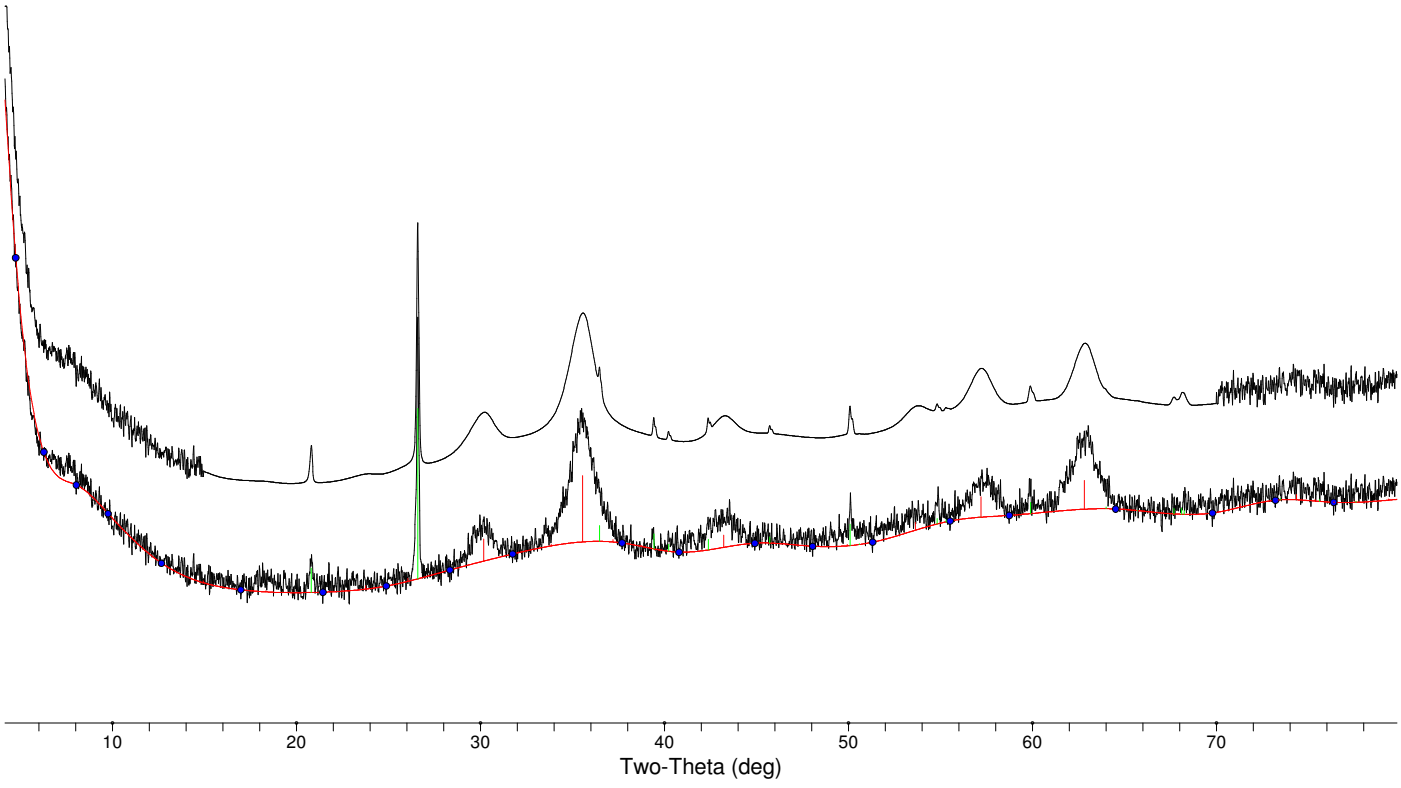
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (2)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#98-000-0369	4.22(0%)	15 (1)	54
Maghemite - $Fe_{21.16}O_{31.92}$	PDF#01-089-5892	4.39(5%)	85 (6)	26

XRF(Wt%): Fe=59%, Si=7%, O=34%

NOTE: Fitting Halted at Iteration 15(4): R=1.05% (E=1.09%, R/E=0.96, P=17, EPS=0.5)





Whole Pattern Fitting and Rietveld Refinement

FILE: [MRP-19498_C-522677_EMIT_BR93-5B.xrdml] BR93-5B Magnetite Skarn, Barstow CA
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=32052, 12/14/21 07:44p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\MRP-19498_C-52...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 4.0 - 76.8(deg)

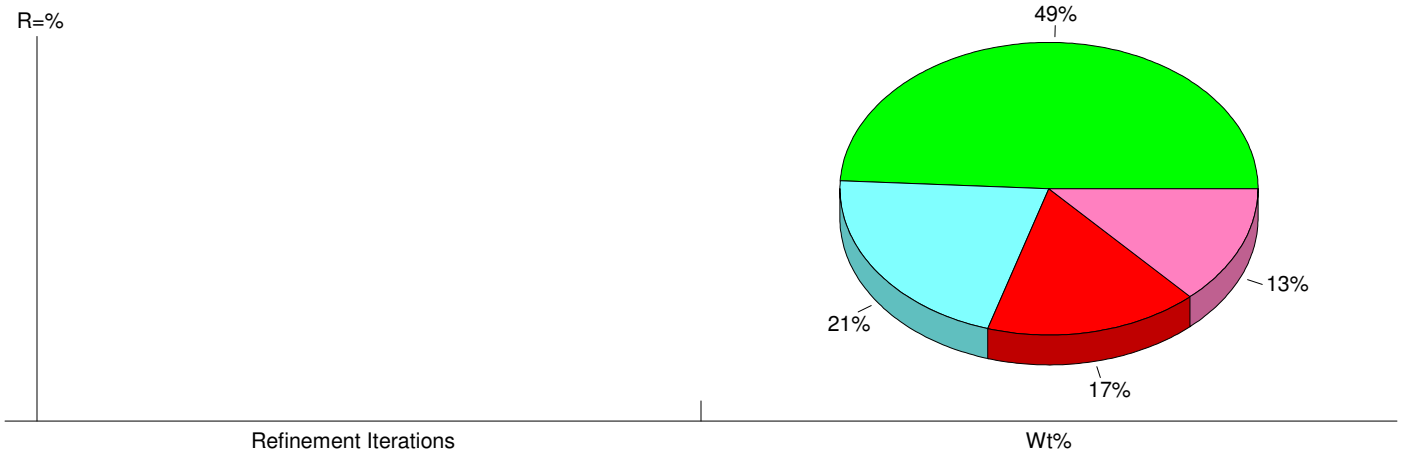
- ☑ Zero Offset of Goniometer - 2Theta = 0.999523(0.063889)
- ☑ Specimen Displacement - Cos(Theta) = -0.970969(0.068589)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

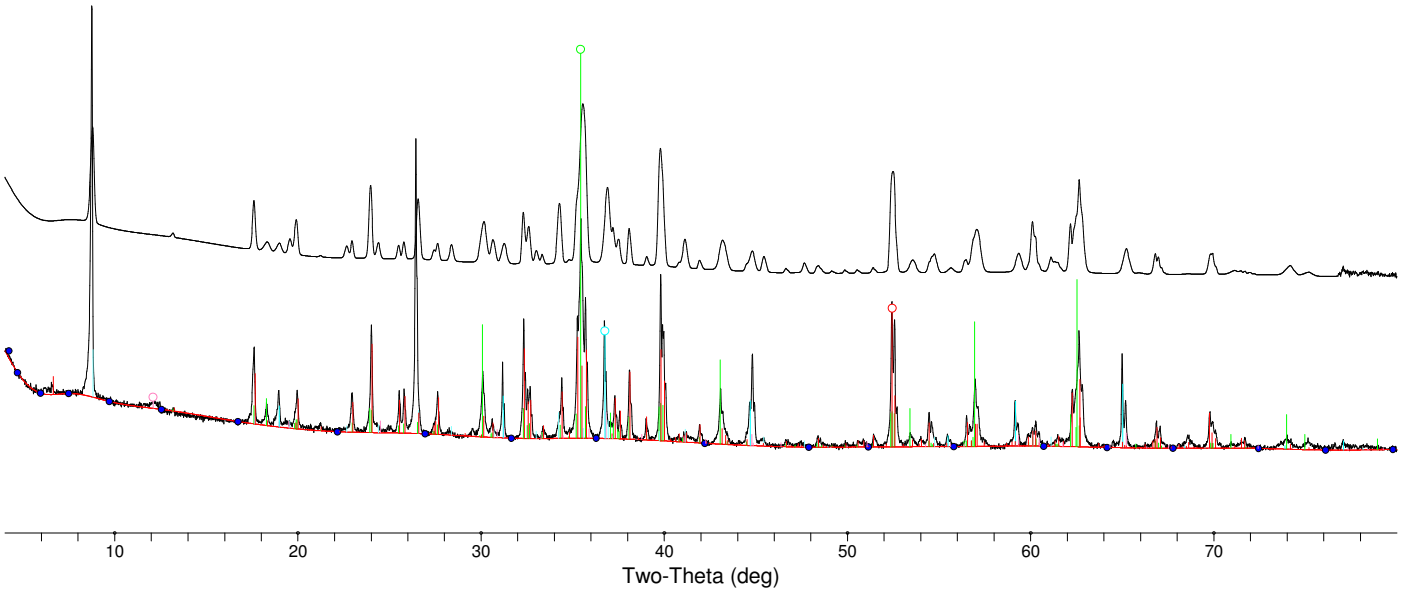
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (4)	Source	I/Ic	Wt%	#L
Hydroxylclinohumite - $Mg_9(SiO_4)_4(OH)_2$	PDF#00-031-0809	0.38(5%)	49 (3)	82
Hendricksite - $KZn_3AlSi_3O_{10}(OH)_2$	PDF#00-027-0468	1.68(5%)	21 (1)	19
Magnetite - Fe_3O_4	PDF#98-000-0294	5.20(0%)	17 (1)	30
Spinel - $(Mg_{0.632}Fe_{0.161}Mn_{0.004}Al_{0.203})(Al_{1.724}Fe_{0.044}Mg_{0.232})O_4$	PDF#01-079-5988	2.02(5%)	13 (1)	12

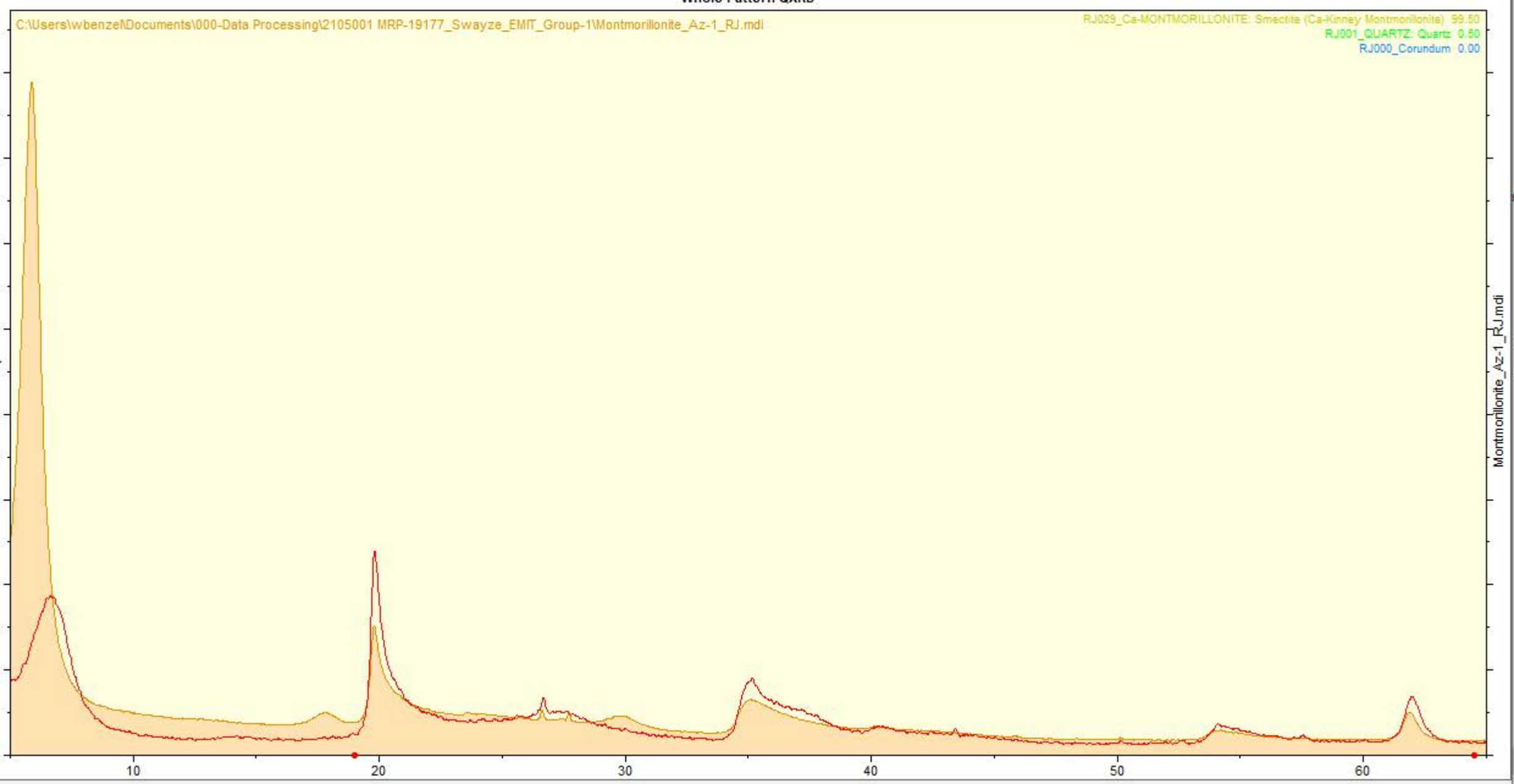
XRF(Wt%): Zn=8%, Fe=13%, Mn=0%, K=2%, Si=12%, Al=6%, Mg=19%, O=41%, H=0%

NOTE: Fitting Halted at Iteration 0(1): R=10.18% (E=1.23%, R/E=8.27, P=14, EPS=0.5)





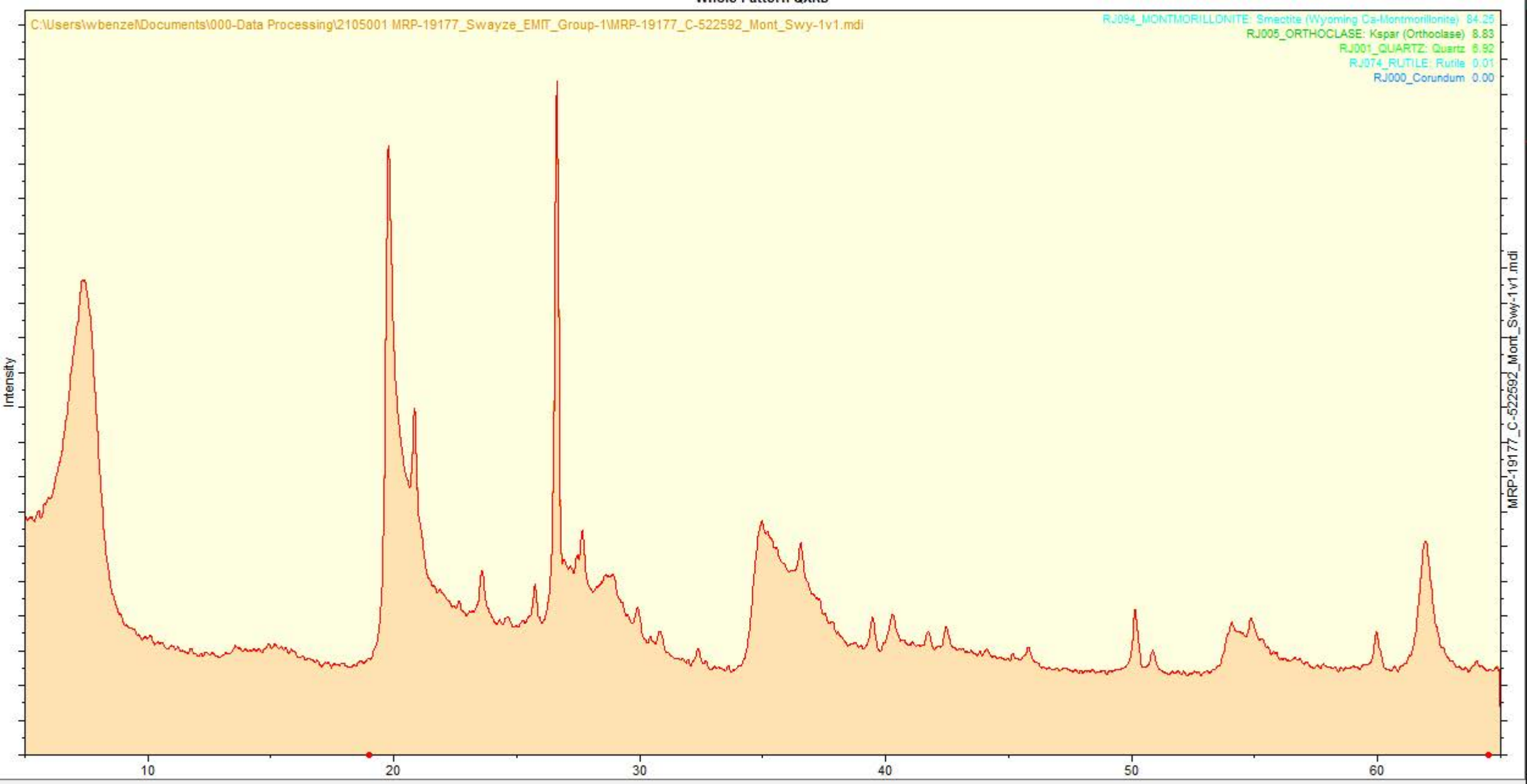
Whole Pattern fitting



(3) MIF [5-65] Al2O3 | 0 | 0.5 | 100 | 12 LSR cycles, Rp=17.88%, d2T=-0.02, Rwp=21.82%

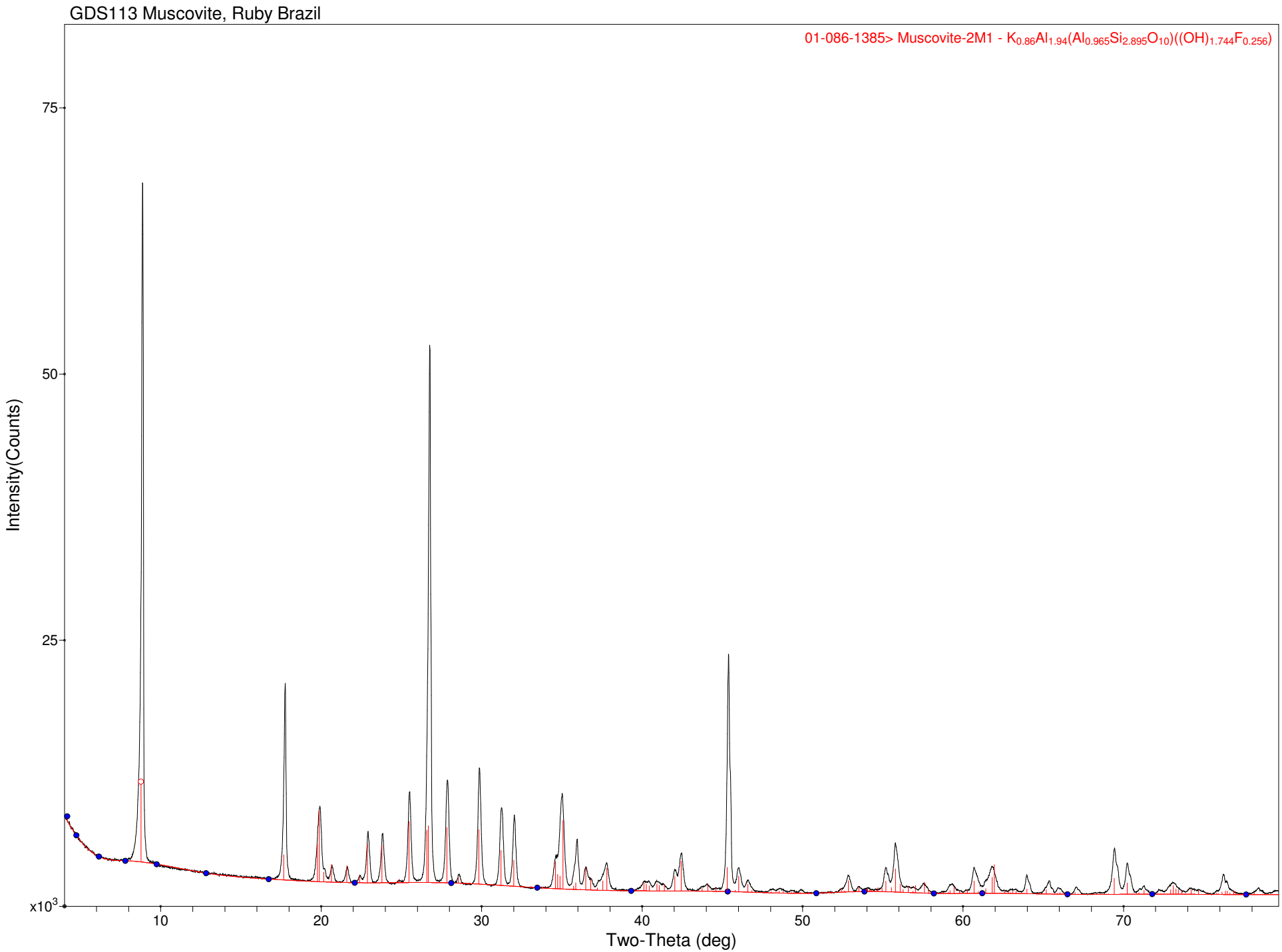
#	Description	Scale	Best w[%]	d2Th	MIF	Rank
☑ 1	RJ000_Corundum	0.6107	0.00	0.00	1	0.27
☑ 29	**RJ029_Ca-MONTMORILLONITE: Smectite (Ca-Ki...**	136.2800	99.50	-0.020	1.568	0.79
☑ 2	**RJ001_QUARTZ: Quartz**	0.7466	0.50	-0.020	1.654	0.29

Whole Pattern Fitting



(3) MIF [5-65] Al2O3 | 0 | 0.5 | 100 | 12 LSR cycles, Rp=0.32%, d2T=-0.06, Rwp=0.5%

#	Description	Scale	Best w[%]	d2Th	MIF	Rank
1	RJ000_Corundum	0.0000	0.00	0.00	1	0.27
94	**RJ094_MONTMORILLONITE: Smectite (Wyomin...**	129.8522	84.25	-0.060	1.498	0.76
6	**RJ005_ORTHOCLASE: Kspar (Orthoclase)**	9.5610	8.83	-0.060	1.683	0.18
2	**RJ001_QUARTZ: Quartz**	9.5395	6.92	-0.060	1.654	0.29
74	RJ074_RUTILE: Rutile	0.0195	0.01	0.01	1.562	0.33


GDS113 Muscovite, Ruby Brazil
01-086-1385> Muscovite-2M1 - $K_{0.86}Al_{1.94}(Al_{0.965}Si_{2.895}O_{10})((OH)_{1.744}F_{0.256})$
75
50
25
x10^3
Intensity(Counts)
10
20
30
40
50
60
70
Two-Theta (deg)

EMIT-Muscovite + Chlorite CU91-253D Cuprite, NV

FILE: [MRP-19496_C-522672_EMIT_CU91-253D.xrdml] Muscovite + Chlorite CU91-253D Cuprite, NV
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=57698, 08/26/21 08:31a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108008_WBSSS-6369_Swayze_EMIT-Group-3\MRP-19496_C-5...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 71.0(deg)

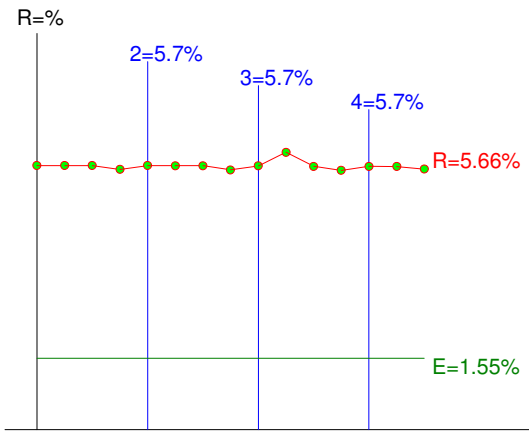
- ☑ Zero Offset of Goniometer - 2Theta = -0.702792(0.152924)
- ☑ Specimen Displacement - Cos(Theta) = 0.662557(0.146921)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

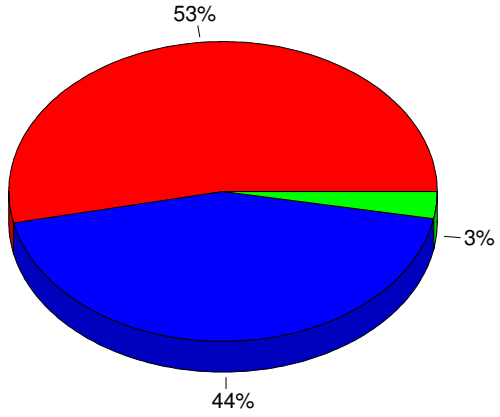
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

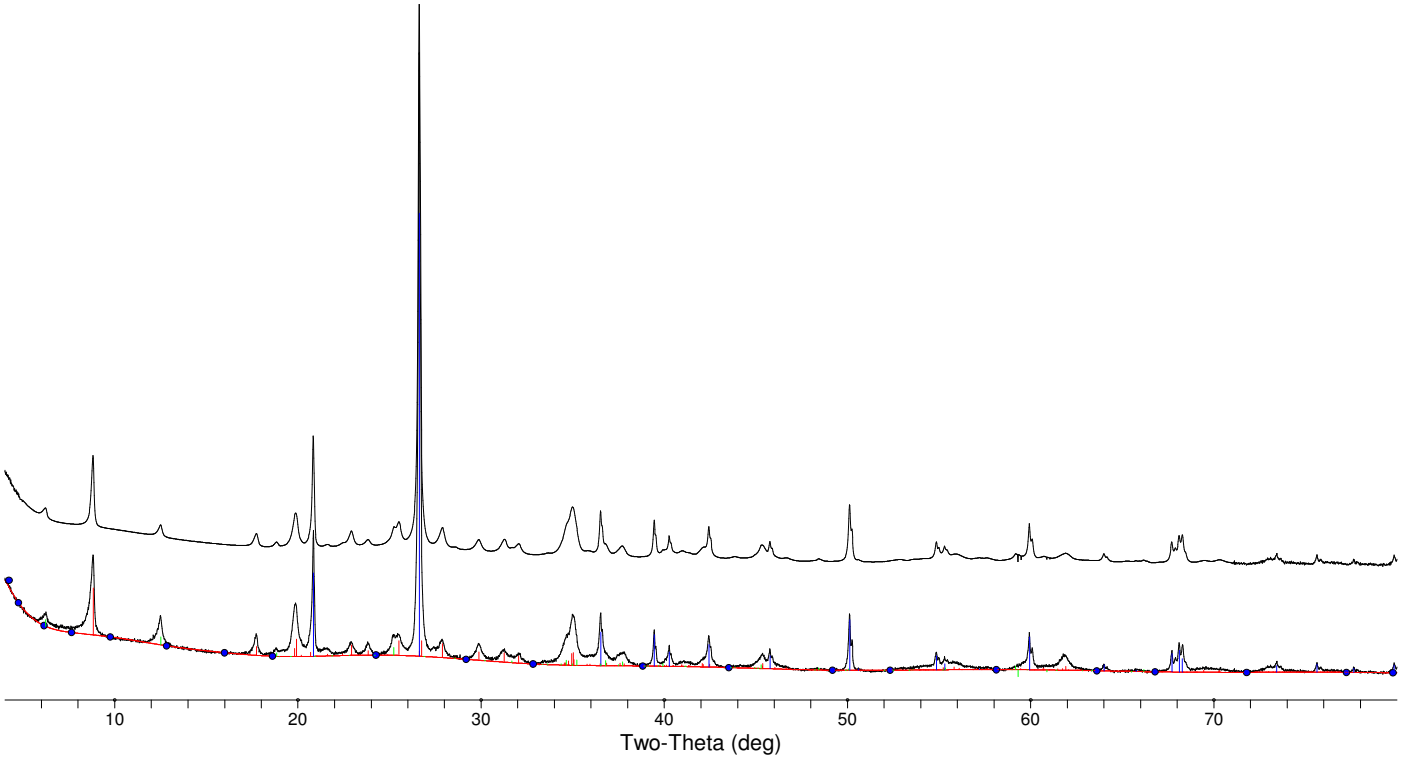
Phase ID (3)	Source	I/Ic	Wt%	#L	PC
Muscovite - $(K_{0.82}Na_{0.18})(Al_{1.97}Fe_{0.03})(AlSi_3O_{10})(OH)_2$	PDF#01-080-0742	0.41(5%)	53 (3)	157	SHF(6,3)
Quartz - SiO_2	PDF#98-000-0369	4.25(0%)	44 (2)	54	<None>
Clinochlore - $(Mg,Al,Fe)_6(Si,Al)_4O_{10}(OH)_8$	PDF#00-046-1323	0.79(5%)	3 (3)	55	SHF(6,3)

XRF(Wt%): Fe=1%, K=4%, Si=32%, Al=11%, Mg=0%, Na=1%, O=50%, H=0%

NOTE: Fitting Halted at Iteration 15(4): R=5.66% (E=1.55%, R/E=3.66, P=33, EPS=0.5)







EMIT-CU93-314 Muscovite-Jarosite Coating

FILE: [CU93-314_Muscovite-Jarosite Coating.mdi] CU93-314 Muscovite-Jarosite Coating
SCAN: 3.0/149.98/0.02/1(sec), Cu, I(p)=38828, 11/23/21 11:05p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\CU93-314_Muscovi...

☑ Allow Negative Isotropic B
☑ Allow Negative Occupancy
☑ Apply Anomalous Scattering
☑ Caglioti's FWHM Function

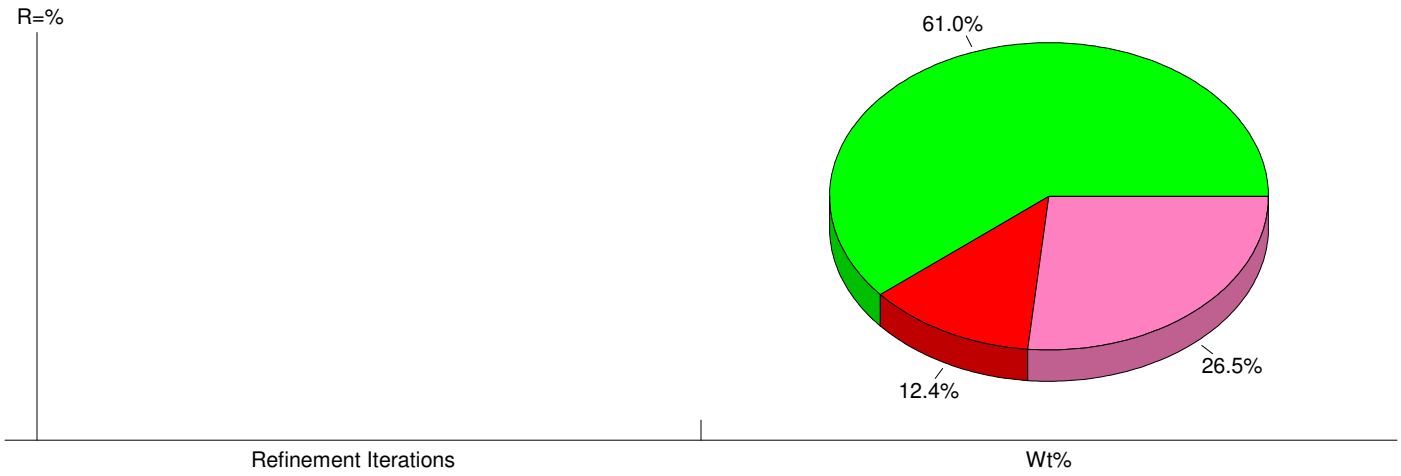
[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 72.5(deg)
☑ Specimen Displacement - Cos(Theta) = -0.069546(0.010454)
☐ Monochromator Correction for LP Factor = 1.0
☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

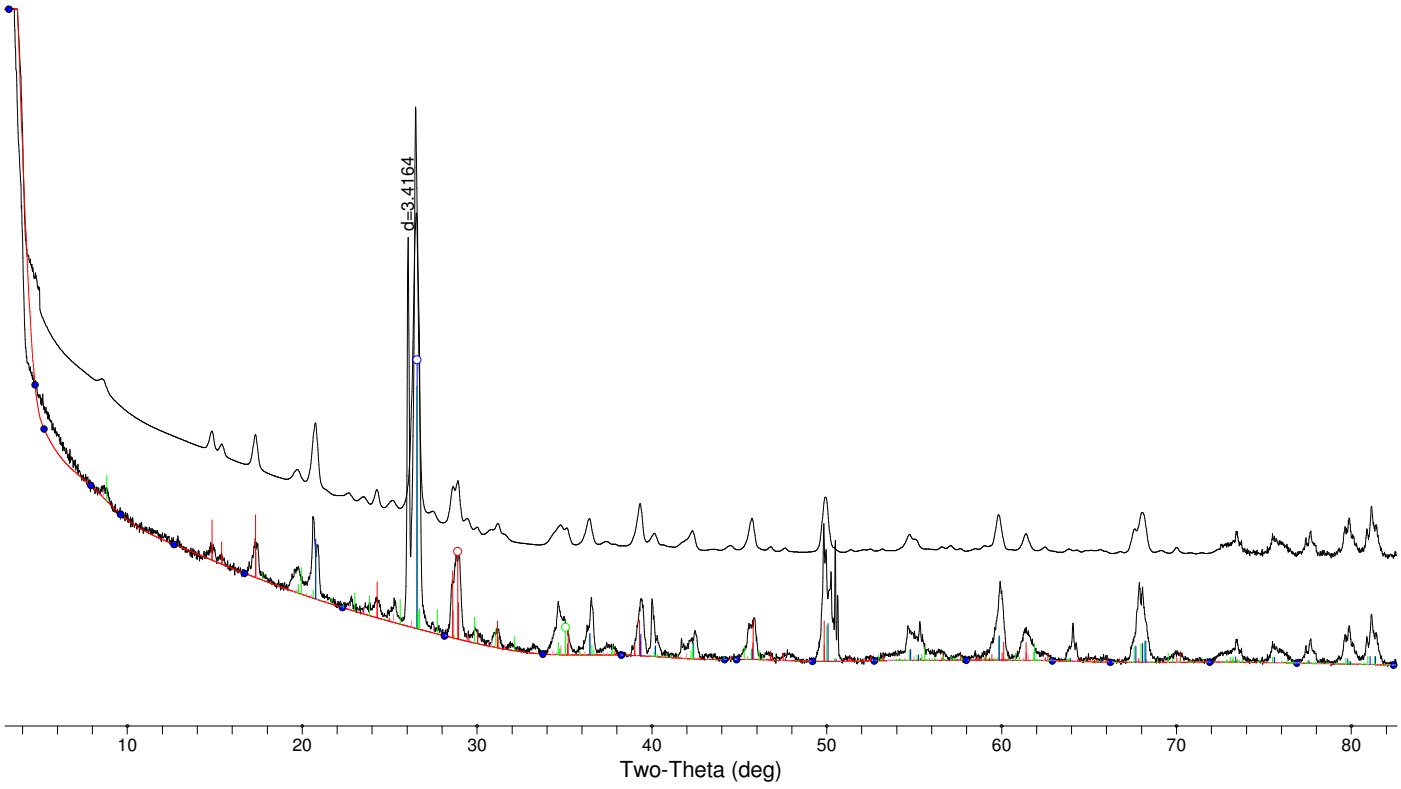
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

Phase ID (3)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#00-033-1161	3.60(5%)	61.0 (3.8)	18
Jarosite - $KFe_3(SO_4)_2(OH)_6$	PDF#00-022-0827	2.20(5%)	12.4 (0.8)	41
Muscovite 2M - $KaI_2[Si_3Al]O_{10}(OH)_2$	PDF#98-000-0321	0.40(0%)	26.5 (1.3)	218

XRF(Wt%): Fe=4.2%, K=3.6%, S=1.6%, Si=34.2%, Al=5.4%, O=50.9%, H=0.1%

NOTE: Fitting Halted at Iteration 0(1): R=11.14% (E=1.61%, R/E=6.9, P=18, EPS=0.5)





EMIT-Low Al-Musc CU91-250A, EMIT-Cuprite, NV

FILE: [MRP-19496_C-522671_EMIT_CU91-250A.xrdml] Low Al-Musc CU91-250A, Cuprite, NV
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=85911, 12/08/21 05:58p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108008_WBSSS-6369_Swayze_EMIT-Group-3\MRP-19496_C-5...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 15.0 - 66.8(deg)

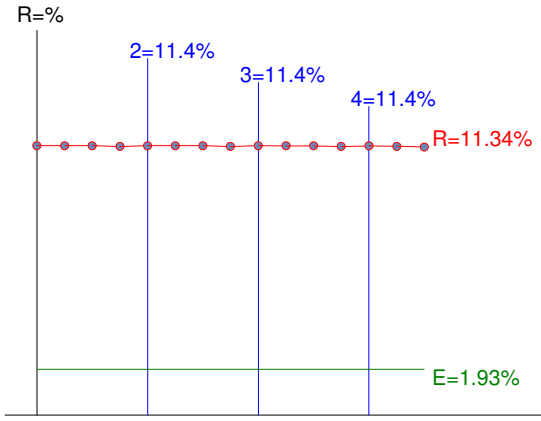
- ☑ Zero Offset of Goniometer - 2Theta = -0.167582(0.023748)
- ☑ Specimen Displacement - Cos(Theta) = 0.189922(0.024866)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

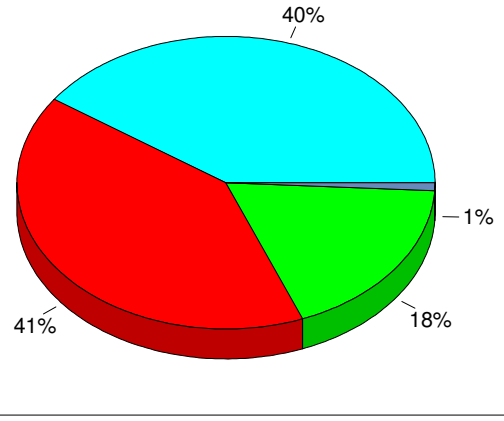
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

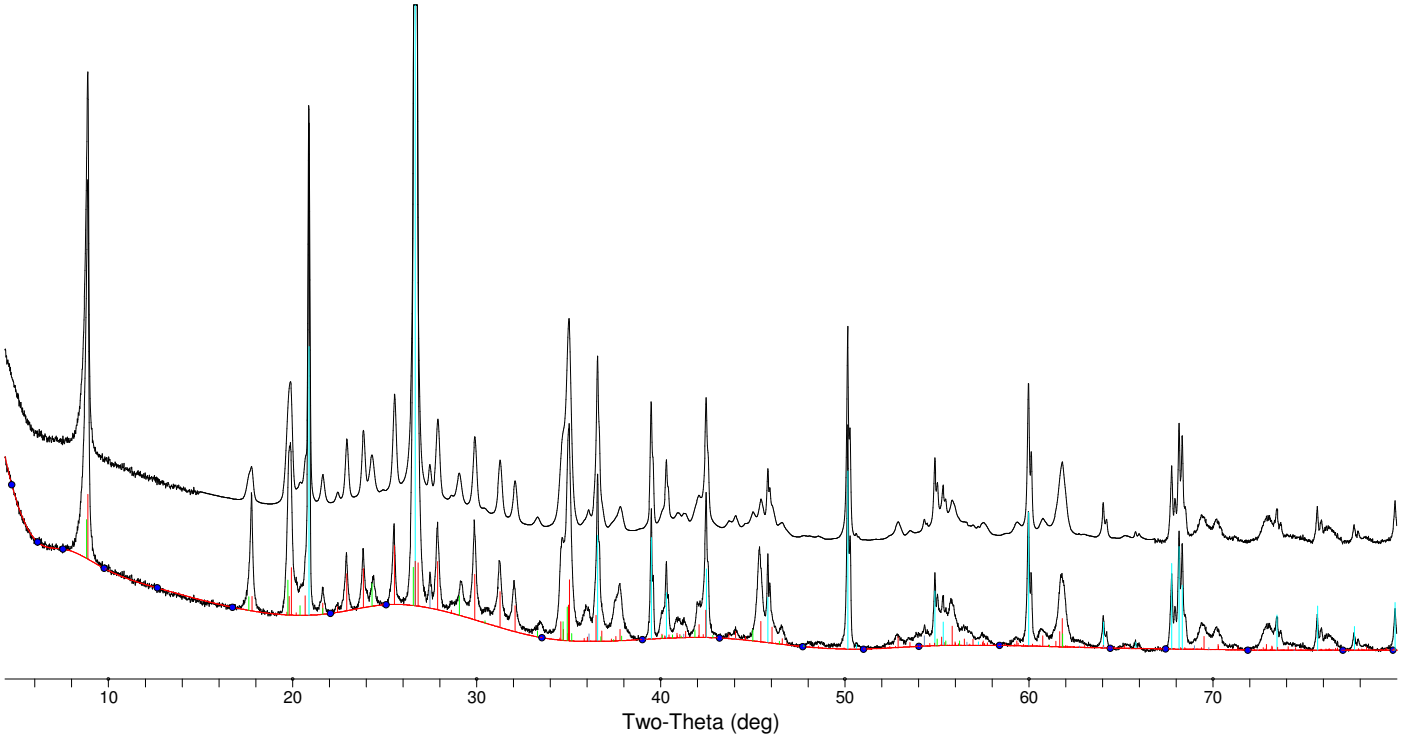
Phase ID (4)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#04-016-2085	4.33(0%)	40 (1)	42
Muscovite - $KAl_3Si_3O_{10}(OH)_2$	PDF#04-017-9606	0.46(0%)	41 (1)	1182
Muscovite - $KAl_2Si_3AlO_{10}(OH)_2$	PDF#00-007-0025	0.80(5%)	18 (1)	28
Rutile - TiO_2	PDF#98-000-0375	3.39(0%)	1 (0)	10

XRF(Wt%): Ti=1%, K=6%, Si=31%, Al=12%, O=50%, H=0%

NOTE: Fitting Halted at Iteration 15(4): R=11.34% (E=1.93%, R/E=5.88, P=18, EPS=0.5)







EMIT-CU93-1 Muscovite Low Al Cuprite NV

FILE: [MRP-19498_C-522678_EMIT_CU93-1.xrdml] CU93-1 Muscovite Low Al Cuprite NV
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=104340, 12/14/21 09:02p
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2109001_MRP-19557_Swayze_EMIT-Group-4\MRP-19498_C-52...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 4.2 - 80.0(deg)

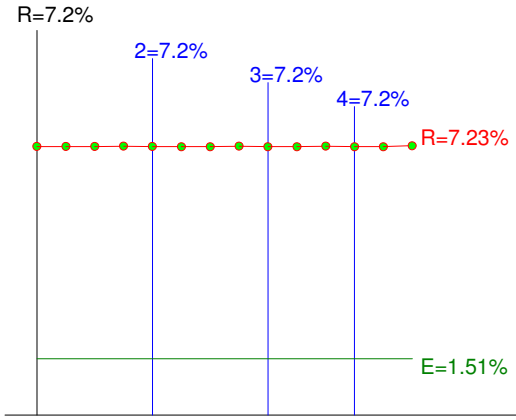
- ☑ Zero Offset of Goniometer - 2Theta = 0.052396(0.008542)
- ☑ Specimen Displacement - Cos(Theta) = -0.043213(0.009019)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

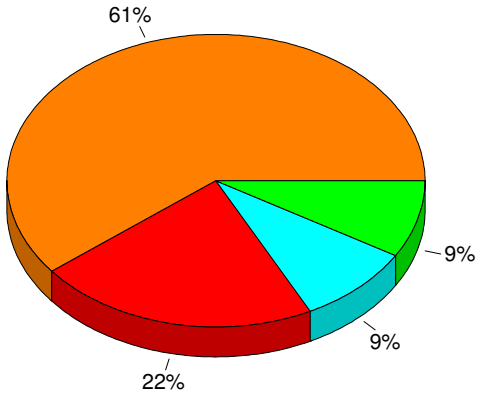
Phase ID (4)	Source	I/Ic	Wt%	#L	PC
Quartz - SiO_2	PDF#98-000-0369	4.22(0%)	61 (1)	68	<None>
Muscovite 2M - $KAl_2[Si_3Al]O_{10}(OH)_2$	PDF#98-000-0321	1.89(0%)	22 (1)	293	(001)=0.564
Calcite - $CaCO_3$	PDF#98-000-0141	2.98(0%)	9 (0)	26	<None>
Clinochlore IIb - $Mg_{4.54}Al_{0.97}Fe_{0.46}Mn_{0.03}(Si_{2.85}Al_{1.15}O_{10})(OH)_8$	PDF#98-000-0165	2.58(0%)	9 (1)	264	SHF(6,3)

XRF(Wt%): Fe=0%, Mn=0%, Ca=4%, K=2%, Si=34%, Al=5%, Mg=2%, O=51%, C=1%, H=0%

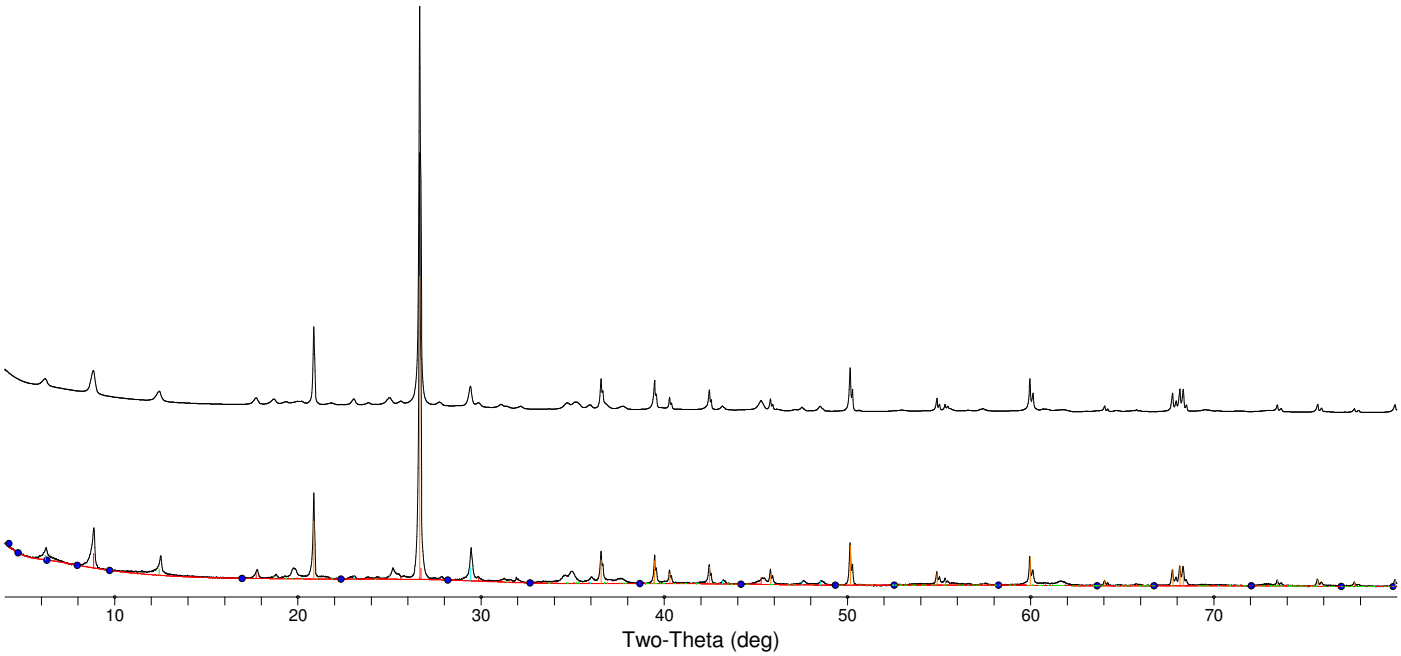
NOTE: Fitting Halted at Iteration 14(4): R=7.23% (E=1.51%, R/E=4.79, P=18, EPS=0.5)



Refinement Iterations



Wt%



EMIT-Med High Al-Muscovite CU91-252D, Cuprite, NV

FILE: [MRP-19496_C-522670_EMIT_CU91-252D.xrdml] Med High Al-Muscovite CU91-252D, Cuprite, NV
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=50778, 08/26/21 05:55a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2108008_WBSSS-6369_Swayze_EMIT-Group-3\MRP-19496_C-5...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.0(deg)

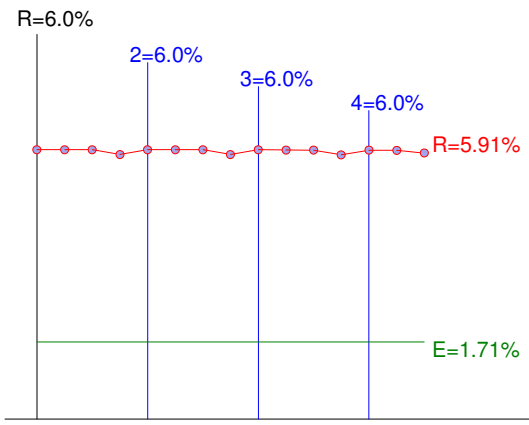
- ☑ Zero Offset of Goniometer - 2Theta = -0.340499(0.019819)
- ☑ Specimen Displacement - Cos(Theta) = 0.296212(0.020874)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

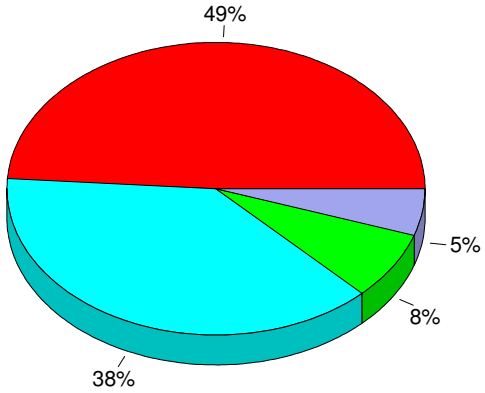
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

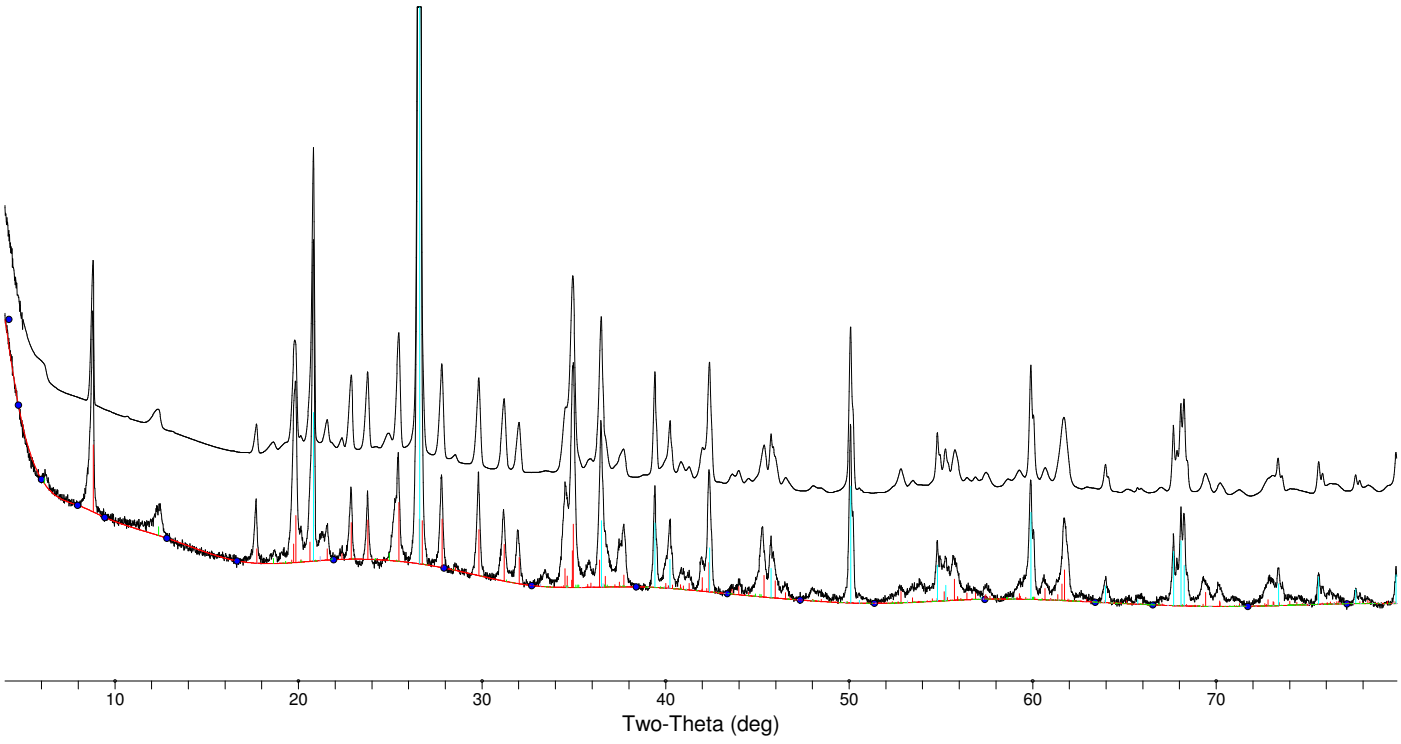
Phase ID (4)	Source	I/Ic	Wt%	#L
Muscovite - $KAl_3Si_3O_{10}(OH)_2$	PDF#04-017-9606	0.46(0%)	49 (1)	1856
Quartz - SiO_2	PDF#04-016-2085	4.35(0%)	38 (0)	70
Clinochlore IIb - $Mg_{4.54}Al_{0.97}Fe_{0.46}Mn_{0.03}(Si_{2.85}Al_{1.15}O_{10})(OH)_8$	PDF#98-000-0165	0.79(0%)	8 (0)	400
Goethite - FeO(OH)	PDF#98-000-0229	2.64(0%)	5 (0)	57

XRF(Wt%): Fe=4%, Mn=0%, K=5%, Si=29%, Al=11%, Mg=1%, O=50%, H=0%

NOTE: Fitting Halted at Iteration 15(4): R=5.91% (E=1.71%, R/E=3.45, P=19, EPS=0.5)







BR93-34B2 Nano-Hematite on Quartzite

FILE: [Clipboard.mdi]
SCAN: 3.2/80.06/0.02/1(sec), Cu, I(p)=4862, 12/14/21 09:48a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2105001 MRP-19177_Swayze_EMIT_Group-1\Clipboard.wpf] [Indi...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 80.1(deg)

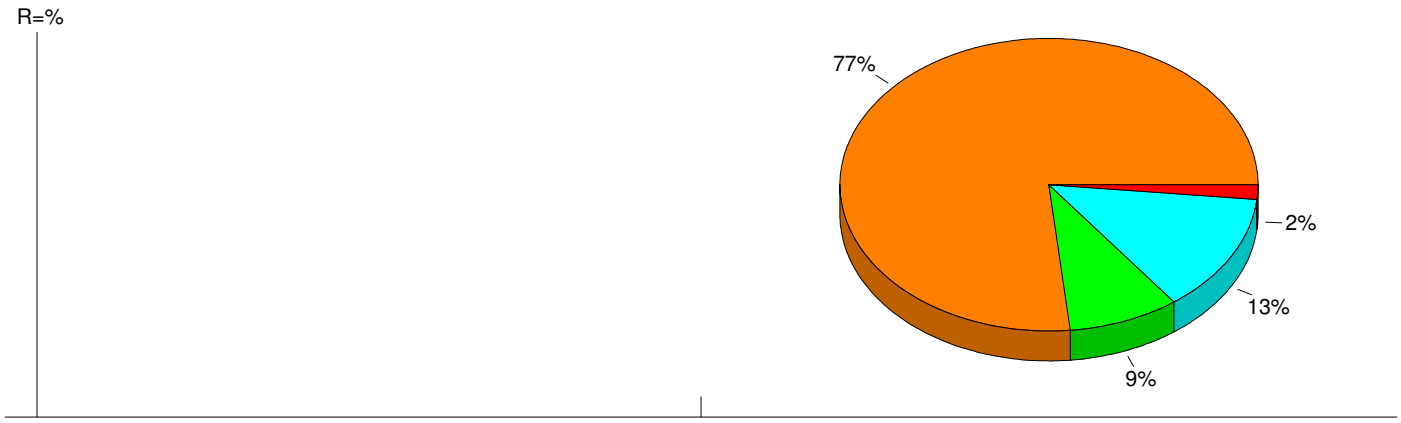
- ☑ Zero Offset of Goniometer - 2Theta = 0.310245(0.039292)
- ☑ Specimen Displacement - Cos(Theta) = -0.442147(0.041241)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

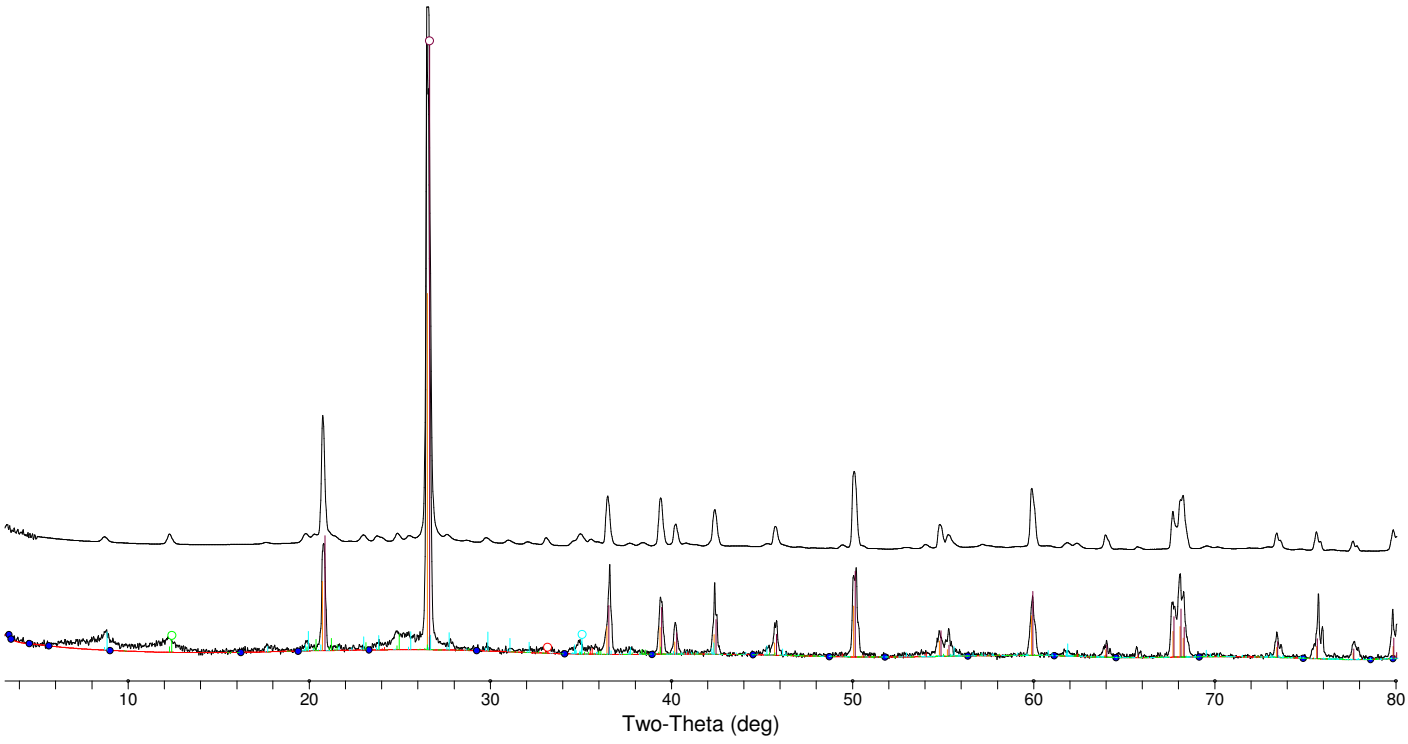
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

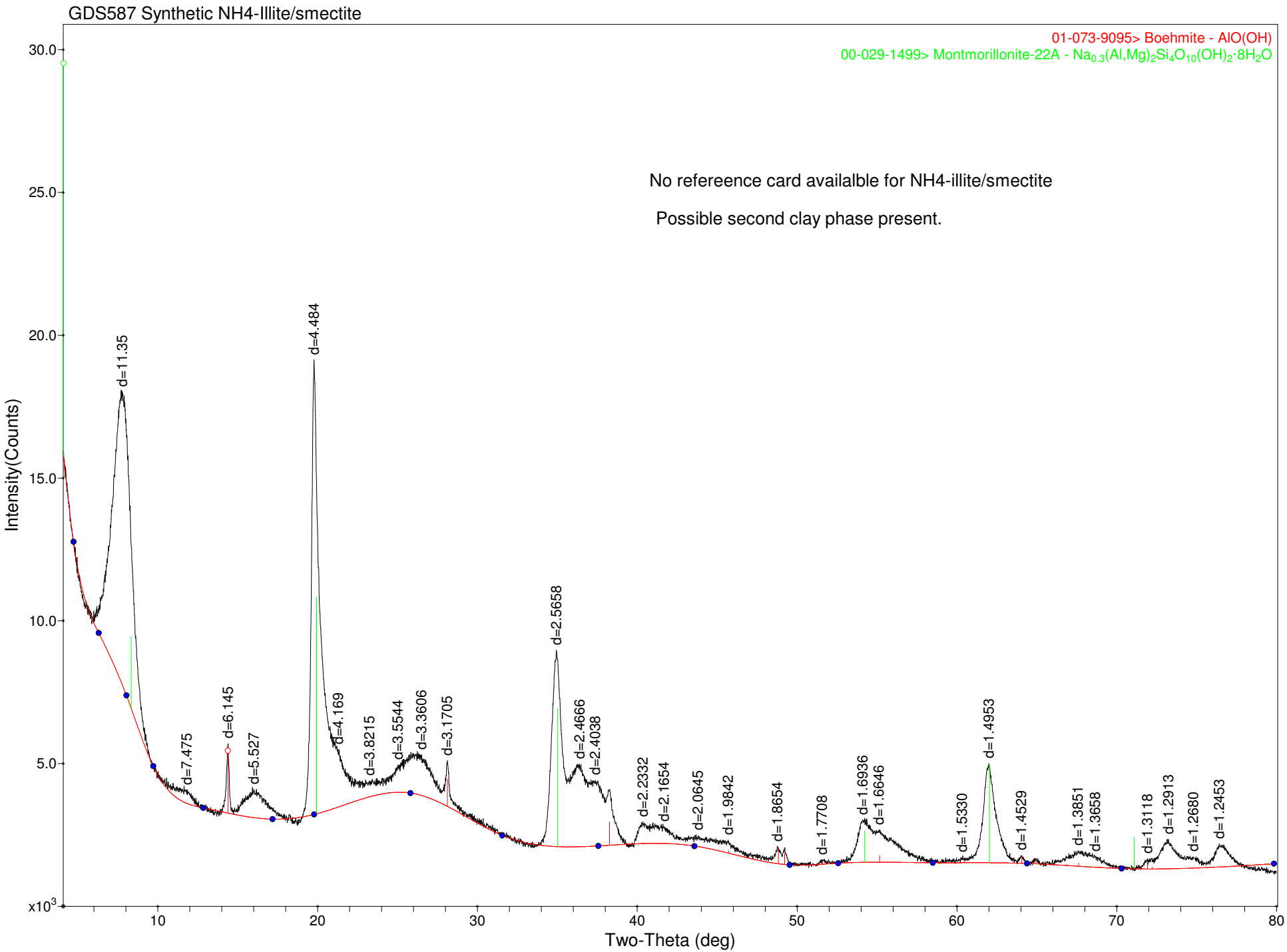
Phase ID (4)	Source	I/Ic	Wt%	#L
Quartz - SiO_2	PDF#98-000-0369	4.26(0%)	77 (1)	70
Kaolinite - $Al_4(OH)_8(Si_4O_{10})$	PDF#98-000-0261	0.87(0%)	9 (1)	775
Muscovite 2M - $KAl_2[Si_3Al]O_{10}(OH)_2$	PDF#98-000-0321	0.40(0%)	13 (1)	296
Hematite - Fe_2O_3	PDF#98-000-0240	3.20(0%)	2 (0)	23

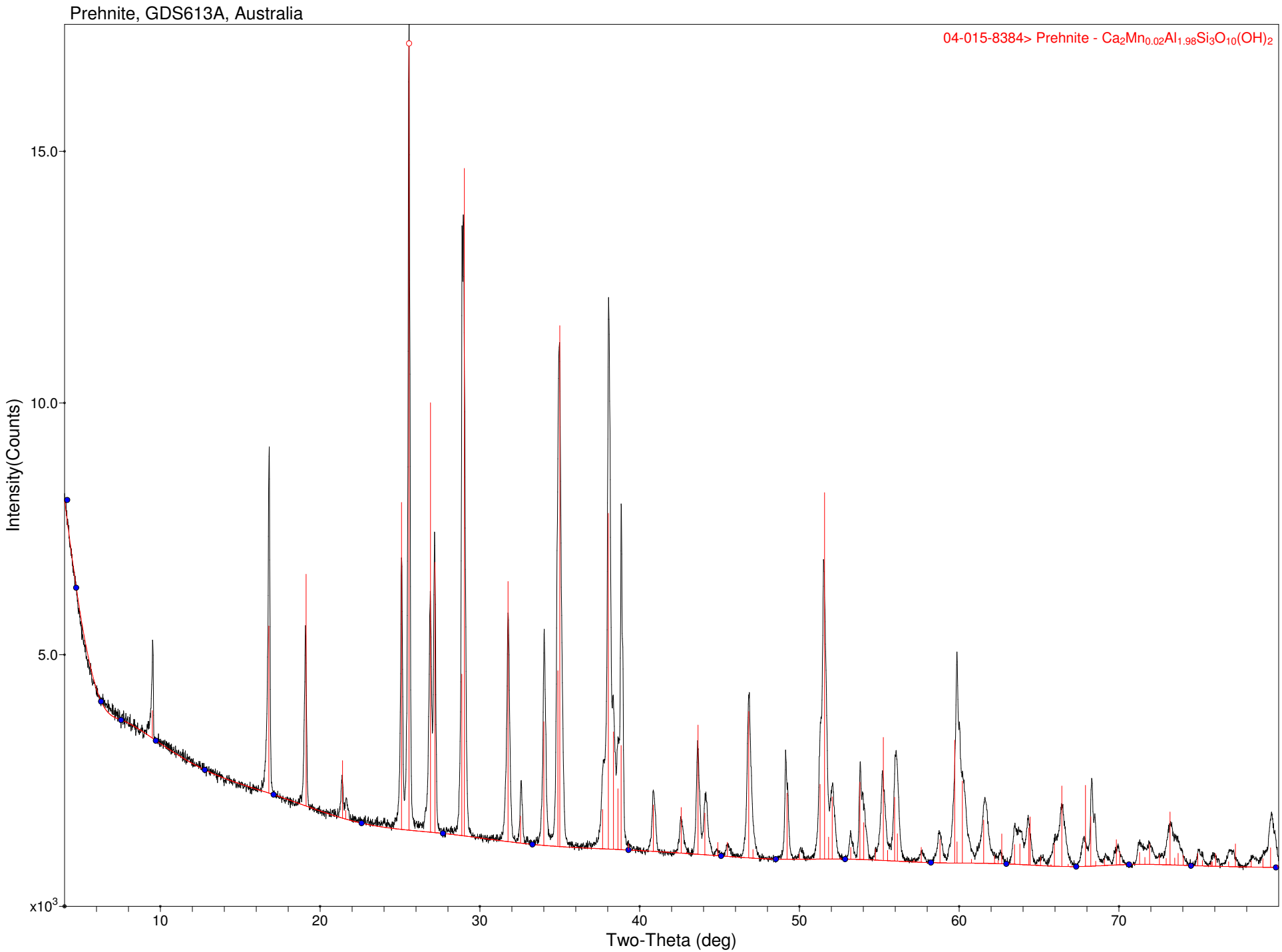
XRF(Wt%): Fe=1%, K=1%, Si=40%, Al=4%, O=52%, H=0%

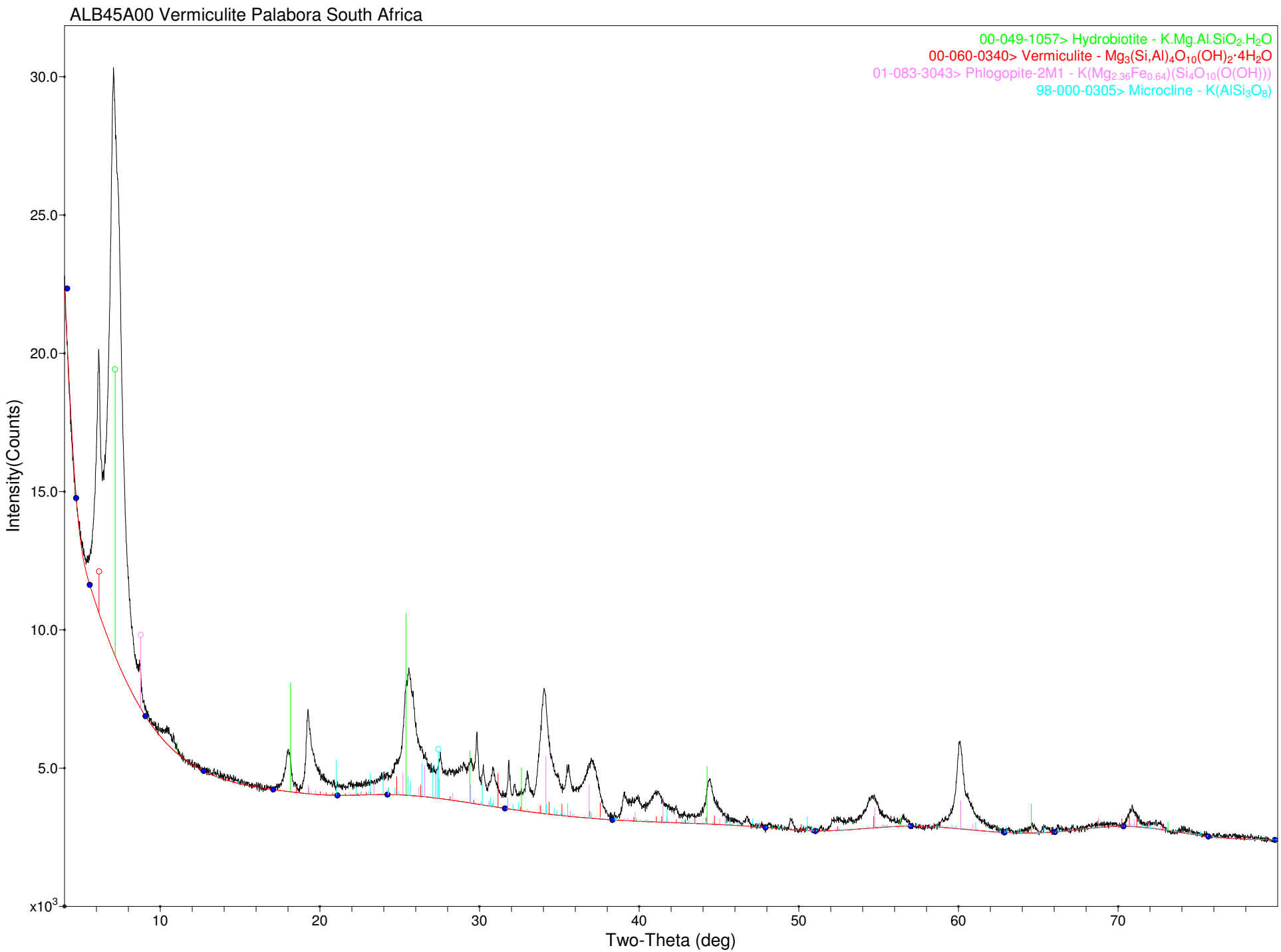
NOTE: Fitting Halted at Iteration 0(1): R=13.2% (E=6.15%, R/E=2.15, P=12, EPS=0.5)






GDS587 Synthetic NH4-Illite/smectite
01-073-9095> Boehmite - AlO(OH)
00-029-1499> Montmorillonite-22A - Na0.3(Al,Mg)2Si4O10(OH)2·8H2O
No refereence card availalble for NH4-illite/smectite
Possible second clay phase present.
Intensity(Counts)
x10^3
Two-Theta (deg)
d=11.35
d=7.475
d=6.145
d=5.527
d=4.484
d=4.169
d=3.8215
d=3.5544
d=3.3606
d=3.1705
d=2.5658
d=2.4666
d=2.4038
d=2.2332
d=2.1654
d=2.0645
d=1.9842
d=1.8654
d=1.7708
d=1.6936
d=1.6646
d=1.5330
d=1.4953
d=1.4529
d=1.3851
d=1.3658
d=1.3118
d=1.2913
d=1.2680
d=1.2453


Prehnite, GDS613A, Australia
04-015-8384> Prehnite - $Ca_2Mn_{0.02}Al_{1.98}Si_3O_{10}(OH)_2$
Intensity(Counts)
15.0
10.0
5.0
x10^3
10
20
30
40
50
60
70
Two-Theta (deg)


ALB45A00 Vermiculite Palabora South Africa
00-049-1057> Hydrobiotite - K.Mg.Al.SiO2.H2O
00-060-0340> Vermiculite - Mg3(Si,Al)4O10(OH)2·4H2O
01-083-3043> Phlogopite-2M1 - K(Mg2.36Fe0.64)(Si4O10(O(OH)))
98-000-0305> Microcline - K(AlSi3O8)
Intensity(Counts)
x10^3
30.0
25.0
20.0
15.0
10.0
5.0
10
20
30
40
50
60
70
Two-Theta (deg)

EMIT-Vermiculite GDS458, Russia

FILE: [MRP-19177_C-522593_Verm_GDS458.xrdml] Vermiculite GDS458, Russia
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=143578, 08/25/21 08:27a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2105001 MRP-19177_Swayze_EMIT_Group-1\MRP-19177_C-522...

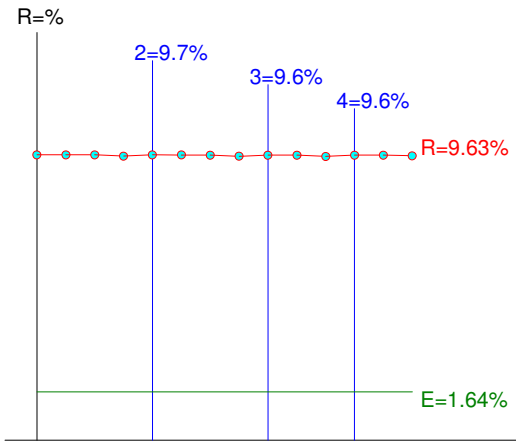
- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering
- [Diffractometer LP] Two-Theta Range of Fit = 10.0 - 79.2(deg)
- ☑ Specimen Displacement - Cos(Theta) = 0.017168(0.011346)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

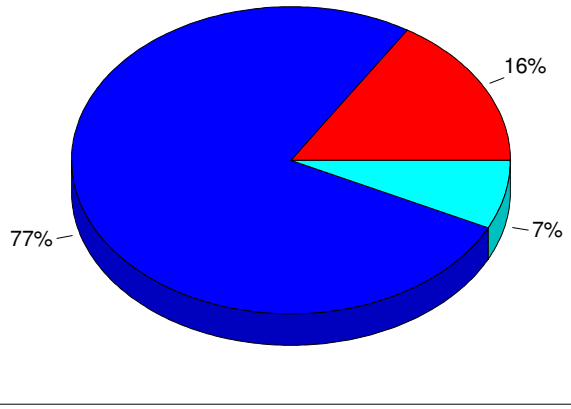
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

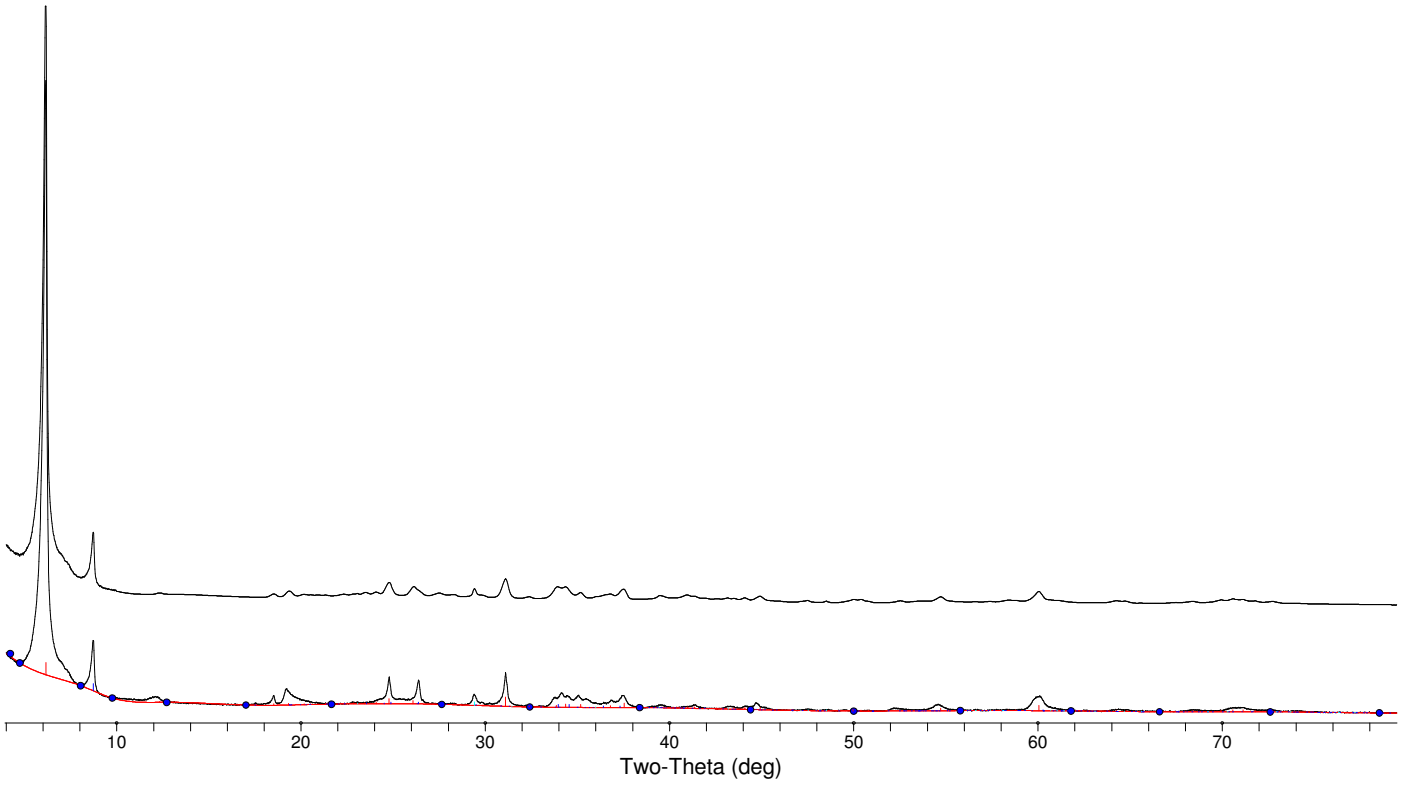
Phase ID (3)	Source	I/Ic	Wt%	#L
Vermiculite - $Mg_3(Si,Al)_4O_{10}(OH)_2 \cdot 4H_2O$	PDF#00-060-0340	10.00(5%)	16 (1)	52
Phlogopite - $K(Mg_{2.36}Fe_{0.64})(Si_4O_{10}(O(OH)))$	PDF#01-083-3043	1.09(5%)	77 (6)	184
Calcite - $CaCO_3$	PDF#98-000-0141	2.99(5%)	7 (1)	24

XRF(Wt%): Fe=6%, Ca=3%, K=7%, Si=22%, Al=2%, Mg=13%, O=46%, C=1%, H=1%

NOTE: Fitting Halted at Iteration 14(4): R=9.63% (E=1.64%, R/E=5.87, P=21, EPS=0.5)







EMIT-WS681 Vermiculite, Kent, CT

FILE: [MRP-19177_C-522595_Verm_WS681.xrdml] WS681 Vermiculite, Kent, CT
SCAN: 4.0084/79.9945/0.01671/125.095(sec), Cu(45kV,40mA), I(p)=14113, 08/25/21 11:02a
PROC: [C:\Users\wbenzel\Documents\000-Data Processing\2105001 MRP-19177_Swayze_EMIT_Group-1\MRP-19177_C-522...

- ☑ K-alpha2 Peak Present
- ☑ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- ☑ Apply Anomalous Scattering

[Diffractometer LP] Two-Theta Range of Fit = 10.0 - 80.0(deg)

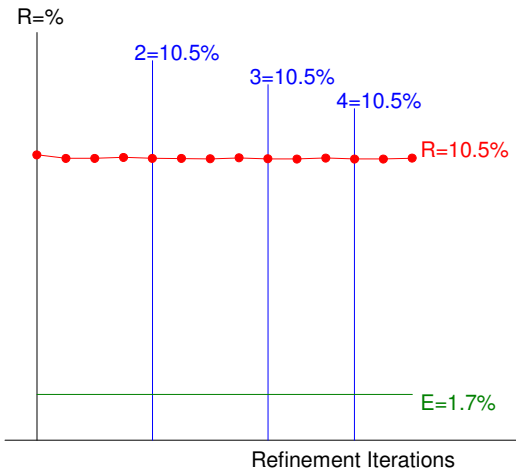
- ☑ Zero Offset of Goniometer - 2Theta = -0.987534(0.175746)
- ☑ Specimen Displacement - Cos(Theta) = 0.930732(0.186938)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

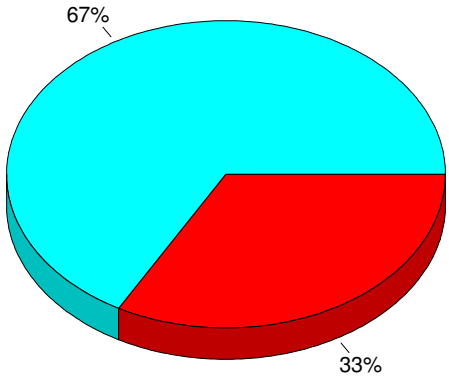
Profile Shape Function (PSF) for All Phases: pseudo-Voigt, Fixed-BG, Lambda=1.54059Å (Cu/K-alpha1)

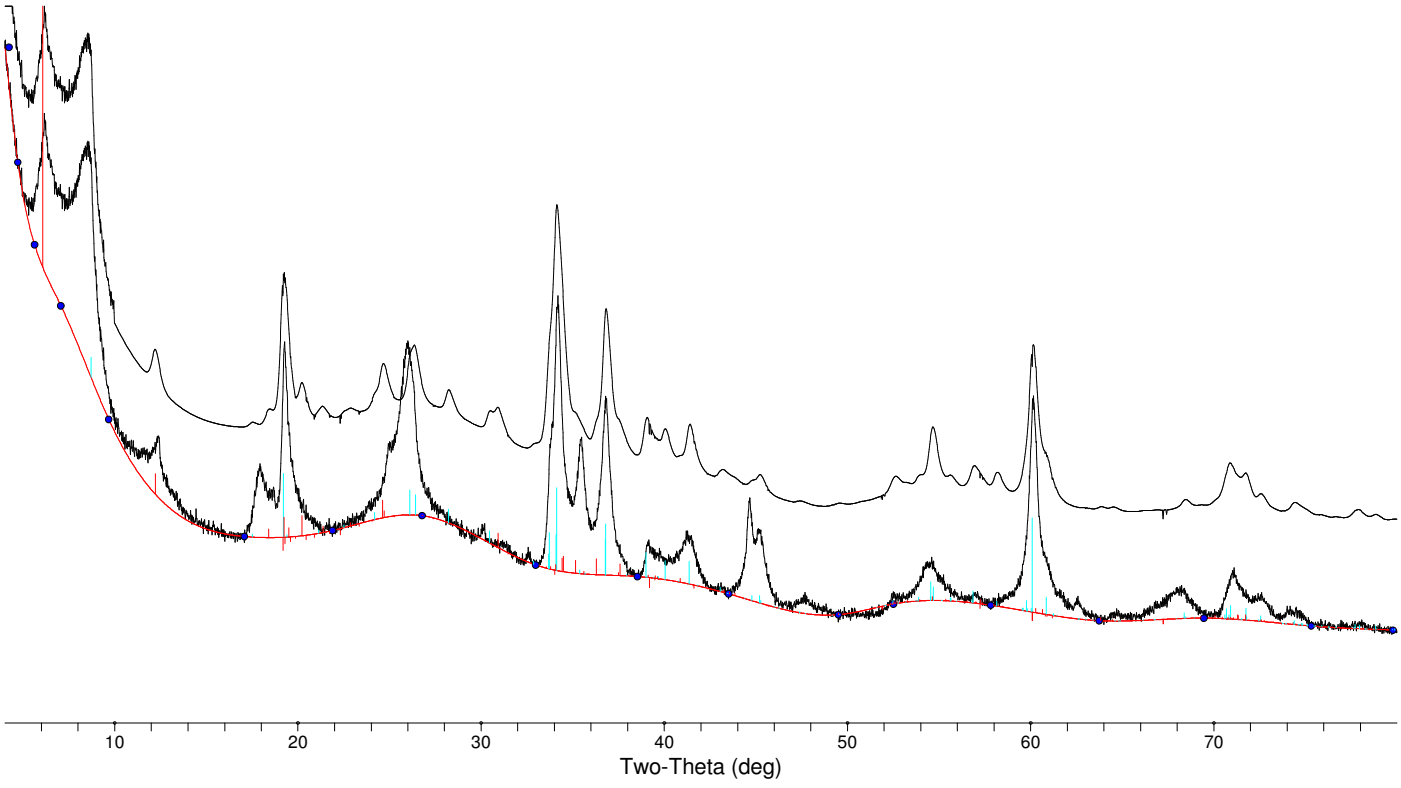
Phase ID (2)	Source	I/Ic	Wt%	#L	PC
Phlogopite - $K_2Mg_6(Al_2Si_6O_{20})(OH)_4$	PDF#01-089-4212	0.46(5%)	67 (6)	141	SHF(6,3)
Vermiculite - $Mg_3(Si_4O_{10})(OH)_2$	PDF#01-074-1732	15.00(5%)	33 (6)	136	SHF(6,3)

XRF(Wt%): K=6%, Si=23%, Al=4%, Mg=18%, O=48%, H=0%

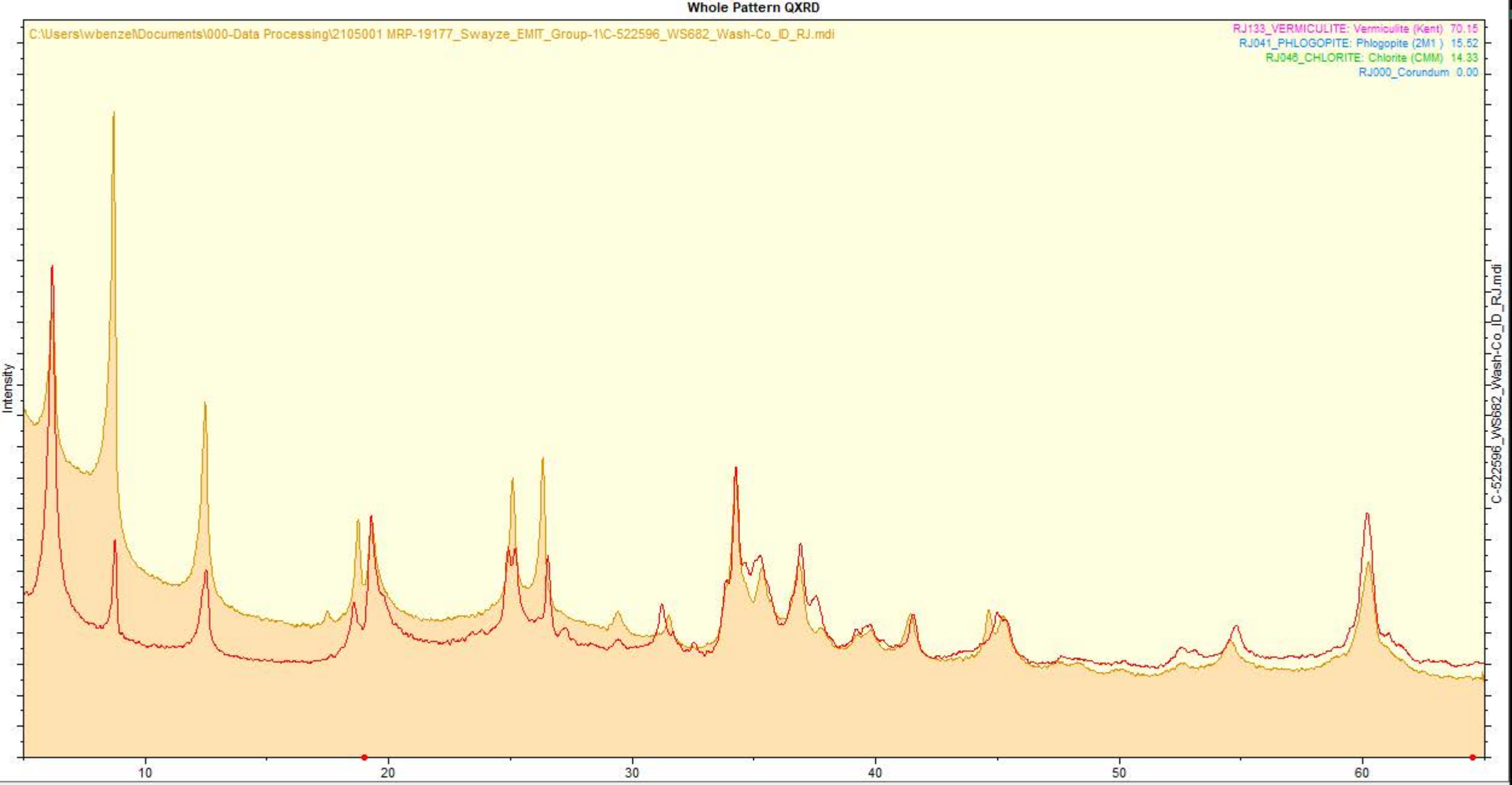
NOTE: Fitting Halted at Iteration 14(4): R=10.5% (E=1.7%, R/E=6.18, P=16, EPS=0.5)







Whole Pattern QXRD



(3) MIF [5-65] Al2O3 | 0 | 0.5 | 100 | 12 LSR cycles, Rp=10.76%, d2T=-0.02, Rwp=13.16%

#	Description	Scale	Best w[%]	d2Th	MIF	Rank
1	RJ000_Corundum	0.0000	0.00	0.00	1	0.27
133	**RJ133_VERMICULITE: Vermiculite (Kent)**	65.3507	**70.15**	-0.020	1.519	0.63
41	**RJ041_PHLOGOPITE: Phlogopite (2M1)**	14.2869	**15.52**	-0.020	1.546	0.28
46	**RJ046_CHLORITE: Chlorite (CMM)**	23.4549	**14.33**	-0.020	1.906	0.50
2	RJ001_QUARTZ: Quartz				1.654	0.29