

Whole Pattern Fitting and Rietveld Refinement

FILE: [std Mumpton Analcime 25606.raw] beige analcime u SCAN: 5.0/65.0/0.03/2.1(sec), Cu, I(p)=6276, 01/14/09 02:30p

PROC: [C:\Documents and Settings\wbenzel\My Documents\AAA Data Processing\901003 Swayze leucite\std Mumpton Analcime...

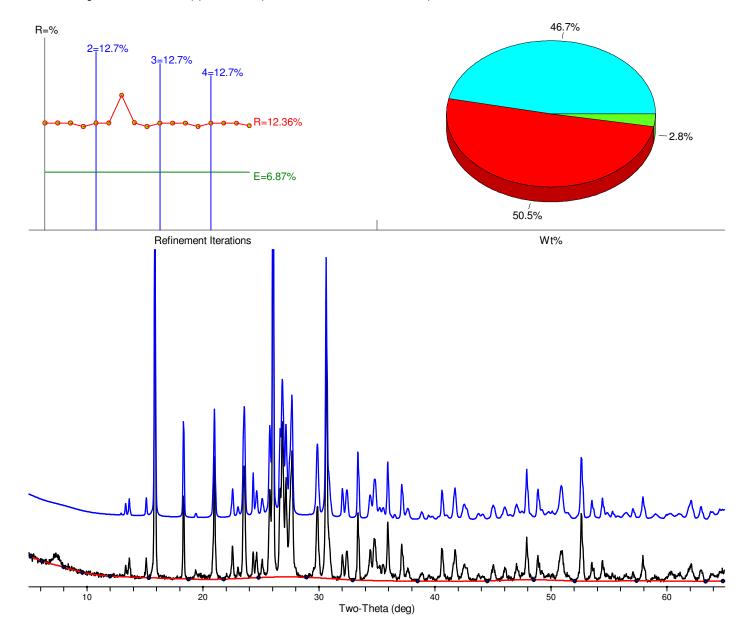
- ✓ K-alpha2 Peak Present
- ✓ Allow Negative Isotropic B
- ☑ Allow Negative Occupancy
- Apply Anomalous Scattering

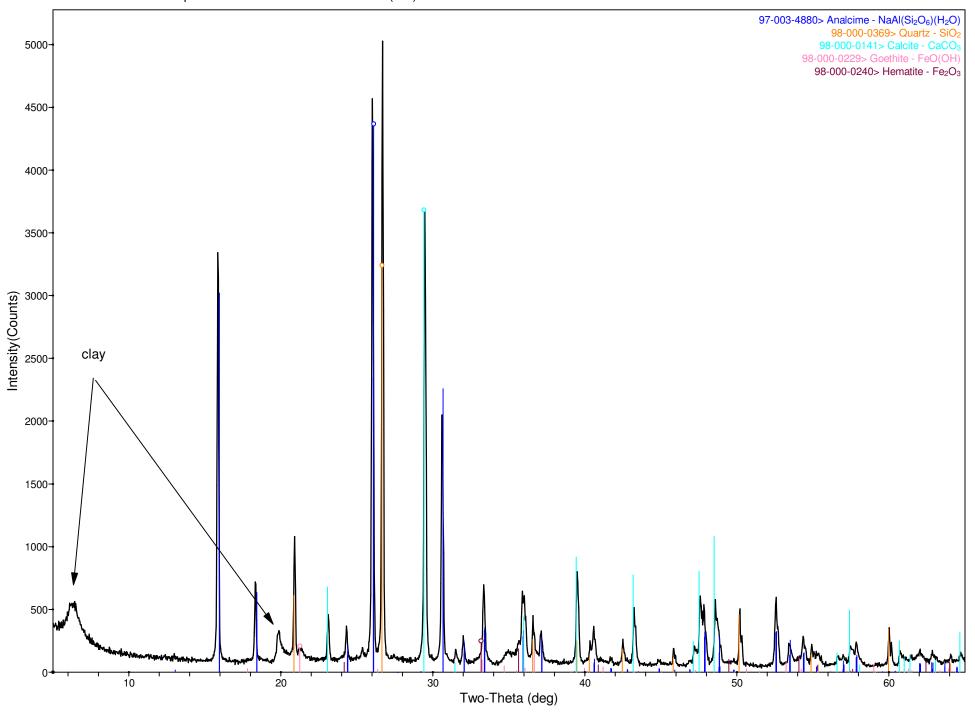
- [Diffractometer LP] Two-Theta Range of Fit = 5.0 65.0(deg)
- Arr Zero Offset of Goniometer 2Theta = -0.178411(0.069264)
- ✓ Specimen Displacement Cos(Theta) = 0.18956(0.071621)
- ☐ Monochromator Correction for LP Factor = 1.0
- ☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

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



NOTE: Fitting Halted at Iteration 17(4): R=12.36% (E=6.87%, R/E=1.8, P=27, EPS=0.5)





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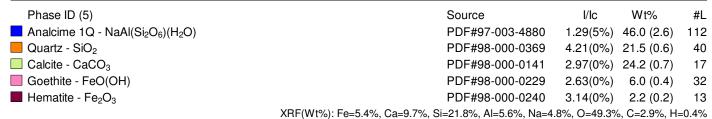
FILE: [std Mumpton Analcime 25607.raw] red analcime u SCAN: 5.0/65.0/0.03/2.1(sec), Cu, I(p)=5026, 01/14/09 12:43p

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 65.0(deg)
- ✓ Zero Offset of Goniometer 2Theta = 0.240454(0.361718)
- \square Specimen Displacement Cos(Theta) = -0.17169(0.336095)
- ✓ Axial Divergence Cot(2Theta) = -0.00624(0.004487)
- ☐ 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(2), Lambda=1.54059Å (Cu/K-alpha1)



NOTE: Fitting Halted at Iteration 24(4): R=17.22% (E=7.24%, R/E=2.38, P=40, EPS=0.5)

