

Whole Pattern Fitting and Rietveld Refinement

FILE: [fx 67 18B.raw] fx67 18B

SCAN: 4.0/70.0089/0.01995/71(sec), Co(35kV,40mA), I(p)=28280, 07/12/13 09:16a

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 = 4.0 - 70.0(deg)

☒ Specimen Displacement - Cos(Theta) = -0.012566(0.002182)

☐ Monochromator Correction for LP Factor = 1.0

☐ K-alpha2/K-alpha1 Intensity Ratio = 0.5

Profile Shape Function (PSF) for All Phases: Pearson-VII, Fixed-BG, Lambda=1.78899Å (Co/K-alpha1)

| Phase ID (9) | Source | I/Ic | Wt% | #L |
|--|-----------------|----------|------------|-----|
| Quartz - SiO ₂ | PDF#04-008-7651 | 5.05(5%) | 55.7 (3.3) | 12 |
| Apatite - Ca ₅ (PO ₄) ₃ F | PDF#00-015-0876 | 1.50(5%) | 25.1 (1.5) | 35 |
| Illite - KAl ₂ (Si ₃ Al)O ₁₀ (OH) ₂ | PDF#00-043-0685 | 0.50(5%) | 6.2 (0.5) | 46 |
| Pyrite - FeS _{1.96} | PDF#01-073-8127 | 2.66(5%) | 4.0 (0.3) | 8 |
| Orthoclase - KAlSi ₃ O ₈ | PDF#99-000-2749 | 0.90(5%) | 3.2 (0.3) | 8 |
| Albite - NaAlSi ₃ O ₈ | PDF#04-007-5092 | 0.63(5%) | 2.4 (0.2) | 146 |
| Calcite - Ca(CO ₃) | PDF#04-007-4388 | 3.25(5%) | 1.5 (0.1) | 12 |
| Dolomite - CaMg(CO ₃) ₂ | PDF#04-008-8657 | 2.51(5%) | 1.1 (0.1) | 14 |
| Natrolite - Na ₂ (Si ₃ Al ₂)O ₁₀ ·2H ₂ O | PDF#98-000-0325 | 0.91(0%) | 0.8 (0.2) | 182 |

XRF(Wt%): Fe=1.9%, Ca=10.8%, K=1.1%, S=2.1%, P=4.6%, Si=29.3%, Al=1.9%, Mg=0.1%, Na=0.3%, F=0.9%, O=46.6%, C=0.3%, H=0.0%

NOTE: Fitting Halted at Iteration 22(4): R=6.64% (E=2.83%, R/E=2.35, P=48, EPS=0.5)

