Whole Pattern Fitting and Rietveld Refinement

FILE: [901003-01 Swayze.raw] leucite from Spectral Database
SCAN: 5.0/65.0/0.03/2.1(sec), Cu, I(p)=2522, 01/14/09 04:16p
PROC: [WPF Control File]

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

[Diffractometer LP] Two-Theta Range of Fit = 5.0 - 65.0(deg)
- ☑ Zero Offset of Goniometer - 2Theta = 0.303338(0.126605)
- ☑ Specimen Displacement - Cos(Theta) = -0.037658(0.133799)
- ☑ Axial Divergence - Cot(2Theta) = 0.005805(0.002381)
- ☐ 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)

Phase ID (3)	Source	I/Ic	Wt%	#L
🟦 Analcime 1Q - $NaAl(Si_2O_6)(H_2O)$	PDF#97-003-4880	1.28(0%)	4.6 (0.3)	118
🟩 Quartz - SiO_2	PDF#98-000-0369	4.13(0%)	1.4 (0.1)	40
🟦 Leucite - $K(Si_2Al)O_6$	PDF#98-000-0369	1.49(0%)	94.0 (0.9)	207

XRF(Wt%): K=16.8%, Si=27.2%, Al=11.0%, Na=0.5%, O=44.4%

NOTE: Fitting Halted at Iteration 14(4): R=13.5% (E=8.92%, R/E=1.51, P=24, EPS=0.5)