

# Whole Pattern Fitting and Rietveld Refinement

FILE: [fx 60 72.raw] fx60 72  
 SCAN: 4.0/70.0089/0.01995/71(sec), Co(35kV,40mA), I(p)=53301, 07/11/13 06:30p  
 PROC: [C:\Documents and Settings\wust\Desktop\fx 67 18A.wpf] [Individual FWHM Curve]

- |  |   |
|--|---|
| <input checked="" type="checkbox"/> K-alpha2 Peak Present      | [Diffractometer LP] Two-Theta Range of Fit = 4.0 - 70.0(deg)                                |
| <input checked="" type="checkbox"/> Allow Negative Isotropic B | <input checked="" type="checkbox"/> Specimen Displacement - Cos(Theta) = 0.021024(0.002006) |
| <input checked="" type="checkbox"/> Allow Negative Occupancy   | <input type="checkbox"/> Monochromator Correction for LP Factor = 1.0                       |
| <input checked="" type="checkbox"/> Apply Anomalous Scattering | <input type="checkbox"/> 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 (7)	Source	I/Ic	Wt%	#L
Quartz - SiO <sub>2</sub>	PDF#04-008-7651	5.05(5%)	76.0 (4.8)	12
Orthoclase - KAlSi <sub>3</sub> O <sub>8</sub>	PDF#99-000-2749	0.90(5%)	9.8 (0.8)	8
Illite - KAl <sub>2</sub> (Si <sub>3</sub> Al)O <sub>10</sub> (OH) <sub>2</sub>	PDF#00-043-0685	0.50(5%)	5.7 (0.5)	46
Albite - NaAlSi <sub>3</sub> O <sub>8</sub>	PDF#04-007-5092	0.63(5%)	2.7 (0.3)	149
Pyrite - FeS <sub>1.96</sub>	PDF#01-073-8127	2.66(5%)	2.4 (0.2)	8
Natrolite - Na <sub>2</sub> (Si <sub>3</sub> Al <sub>2</sub> )O <sub>10</sub> ·2H <sub>2</sub> O	PDF#98-000-0325	0.91(0%)	1.8 (0.2)	186
Calcite - Ca(CO <sub>3</sub> )	PDF#04-007-4388	3.25(5%)	1.6 (0.1)	12

XRF(Wt%): Fe=1.1%, Ca=0.6%, K=1.9%, S=1.3%, Si=41.0%, Al=2.6%, Na=0.4%, O=50.7%, C=0.2%, H=0.0%

NOTE: Fitting Converged at Iteration 23(4): R=7.59% (E=2.68%, R/E=2.83, P=41, EPS=0.5)

