

# Whole Pattern Fitting and Rietveld Refinement

FILE: [fx 73 70.raw] fx73 70

SCAN: 4.0/70.0089/0.01995/71(sec), Co(35kV,40mA), I(p)=37697, 07/11/13 07:28p

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) = 0.065556(0.002623)

☐ 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 (8)	Source	I/Ic	Wt%	#L
Quartz - SiO <sub>2</sub>	PDF#04-008-7651	5.05(5%)	57.6 (3.5)	12
Orthoclase - KAlSi <sub>3</sub> O <sub>8</sub>	PDF#99-000-2749	0.90(5%)	15.8 (1.3)	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%)	11.1 (0.8)	46
Pyrite - FeS <sub>1.96</sub>	PDF#01-073-8127	2.66(5%)	7.2 (0.5)	8
Albite - NaAlSi <sub>3</sub> O <sub>8</sub>	PDF#04-007-5092	0.63(5%)	3.4 (0.3)	149
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	0.90(0%)	2.3 (0.2)	184
Calcite - Ca(CO <sub>3</sub> )	PDF#04-007-4388	3.25(5%)	1.3 (0.2)	12
Dolomite - CaMg(CO <sub>3</sub> ) <sub>2</sub>	PDF#04-008-8657	2.51(5%)	1.2 (0.2)	14

XRF(Wt%): Fe=3.4%, Ca=0.8%, K=3.3%, S=3.8%, Si=35.7%, Al=4.5%, Mg=0.2%, Na=0.6%, O=47.4%, C=0.3%, H=0.1%

NOTE: Fitting Halted at Iteration 24(4): R=8.31% (E=2.5%, R/E=3.32, P=43, EPS=0.5)

