

Analysis of standards mixtures of known composition

The only way to confirm the accuracy and precision of a technique applied to natural samples is to check against synthetic mixtures of appropriate mineral standards. At X-ray Mineral Services we are continuously improving our methodologies and check our precision and accuracy against mixtures of known mineral standards.

The latest mixtures were prepared to check the quantification given by the Rietveld software BGMN Autoquan, with special interest in the relative proportions of illite and mica.

Illite and mica are structurally similar - their basal reflections have the same 2d spacing. Therefore, it is very difficult to differentiate between them by XRD using a conventional method like the Reference Intensity Ratio (RIR) method. The quantification of illite and mica was therefore achieved using the Rietveld method which is able to decipher experimental complications, such as peak overlap. Being a “full-pattern analysis” method, all intensity data from the pattern are taken into account, resulting in advantages over the conventional RIR method.

In this validation project, most of the minerals were quantified within 1 wt.% absolute error. The relative proportions of illite and mica quantified by Rietveld generally correspond to the known proportions of the two minerals in the mixtures. The biggest errors in the quantification is in the more abundant minerals. This errors are affected by the sums of the errors in the quantification of the less abundant phases.

		Actual	Calculated			Actual	Calculated
Illite	Mix1	6.1	6.0	Calcite	Mix1	5.2	4.8
	Mix2	3.6	3.8		Mix2	10.2	10.6
	Mix3	1.9	2.4		Mix3	11.3	11.3
	Mix4	1.4	1.2		Mix4	1.2	1.4
	Mix5	13.5	10.8		Mix5	1.0	0.8
Muscovite	Mix1	2.9	3.0	Dolomite	Mix1	0.0	0.0
	Mix2	14.1	11.2		Mix2	5.1	6.1
	Mix3	2.2	1.4		Mix3	2.4	3.1
	Mix4	0.5	0.2		Mix4	7.9	8.1
	Mix5	7.6	7.8		Mix5	6.3	6.1
Kaolinite	Mix1	4.9	5.8	Halite	Mix1	0.8	0.6
	Mix2	3.8	4.4		Mix2	0.5	TR
	Mix3	1.7	1.8		Mix3	0.0	0.0
	Mix4	1.0	1.3		Mix4	0.0	0.0
	Mix5	7.6	9.7		Mix5	0.0	0.0
Chlorite	Mix1	0.0	0.0	Barite	Mix1	1.5	TR
	Mix2	0.0	0.0		Mix2	0.7	TR
	Mix3	1.9	2.0		Mix3	0.0	0.0
	Mix4	1.5	2.0		Mix4	0.0	0.0
	Mix5	5.0	5.1		Mix5	0.0	0.0
Quartz	Mix1	68.8	71.1	Anatase	Mix1	1.1	0.9
	Mix2	54.3	57.2		Mix2	1.2	1.1
	Mix3	75.1	75.6		Mix3	0.6	0.4
	Mix4	81.6	80.8		Mix4	1.0	0.7
	Mix5	52.2	53.5		Mix5	0.2	0.0
K-feldspar	Mix1	4.0	2.2	Pyrite	Mix1	1.1	1.1
	Mix2	2.5	1.5		Mix2	2.7	2.5
	Mix3	1.6	1.0		Mix3	1.2	1.0
	Mix4	1.0	0.9		Mix4	0.5	0.4
	Mix5	1.7	1.9		Mix5	4.7	4.5
Plagioclase	Mix1	3.6	4.5		<1	TR=<0.5%	
	Mix2	1.2	1.6		1-2		
	Mix3	0.1	TR		2-3		
	Mix4	2.6	3.1		3-5		
	Mix5	0.1	TR		>5		

