
X-ray Powder Diffraction Rietveld Characterization of Synthetic Aluminum-Substituted Goethite

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Abstract: Rietveld X-ray powder diffraction (XRD) analysis has been evaluated as a procedure for characterizing Al-substituted goethite according to the Rietveld scale factor, unit-cell parameters, and atom positional parameters. The study was conducted with three synthetic goethite samples for which the degree of Al substitution for Fe determined by chemical analysis was 8.0 ± 0.4 , 12.0 ± 0.4 , and 20.1 ± 0.4 mole %. The weight fractions of crystalline material (WFCM) in the specimens, determined from the Rietveld scale factors after correcting for adsorbed water and impurities, were 0.878 (esd = 0.014), 0.919 (0.014), and 0.965 (0.015), respectively. The Al mole % substitutions, inferred from the Rietveld cell parameters according to the method of Schulze (1984), were 10.4 ± 2.5 , 16.5 ± 2.6 , and 17.1 ± 2.6 , respectively. The cause of the significant difference between the second value and the chemical analysis result is not known. The atom positional parameters did not differ significantly within the sample suite and agreed satisfactorily with literature values. The results have demonstrated the value of using Rietveld XRD analysis to determine simultaneously the WFCM and Al mole % substitutions, as well as to confirm the non-hydrogen atom positions.

Key Words: Aluminum • Crystallinity • Goethite • Rietveld refinement • X-ray powder diffraction

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