
The Influence of Aluminum on Iron Oxides. Part XVI: Hydroxyl and Aluminum Substitution in Synthetic Hematites

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Abstract: Synthetic hematites with Al substitutions between 0 and 18 mol % were synthesized at different temperatures and water activities. The cell-edge lengths a for different synthesis conditions decreased linearly with increasing Al substitution. The regression lines, however, had different slopes and intercepts: the series with the highest synthesis temperature (1270 K) had the most negative slope. With increasing Al substitution, the hematites contained increasing amounts of non-surface water. Significant correlations were found between these chemically determined water contents and the deviations of the unit-cell parameters a , c , and V relative to the corresponding 1270 K regression lines. To explain the measured X-ray peak intensities, structural OH had to be included into the theoretical calculations. From intensity ratios normalized to I_{113} , it is possible to determine the structural OH separately from the Al substitution, which can be assessed by the shift of the cell-edge lengths relative to the 1270 K regression lines. The incorporation of Al and OH into the hematite structure induces strain, which was quantified by X-ray diffraction.

Key Words: Al substitution • Cell-edge lengths • Hematite • LOI • OH substitution • X-ray intensity

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