
The Influence of Aluminum on Iron Oxides. VIII. Unit-Cell Dimensions of Al-Substituted Goethites and Estimation of Al From Them

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Abstract: The unit-cell dimensions of synthetic, Al-substituted goethites showed that the *c* dimension is a linear function of Al substitution in the range 0– 33 mole % Al, but that the *a* dimension is variable over this same range. The *b* dimension is also linearly related to Al substitution but is slightly more variable than the *c* dimension for Al substitutions of 20– 33 mole %. The variability of the *a* dimension is postulated to be the result of structural defects. An improved procedure for estimating Al substitution from x-ray powder diffraction positions requires (1) calculation of the *c* dimension from the positions of the 110 and 111 diffraction lines using the formula: $c = (1/d(111)^2 - 1/d(110)^2)^{-1/2}$, and (2) estimation of Al substitution from the relationship: mole % Al = 1730 – 572.0*c*. The 95% confidence interval of the estimate is ± 2.6 mole % Al when using this procedure, in contrast to ± 4.0 mole % Al when the position of the 111 reflection alone is used.

Key Words: Aluminum • Goethite • Iron • Unit-cell dimensions • X-ray powder diffraction

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