

American Mineralogist, Volume 82, pages 44–50, 1997

Fivefold-coordinated Ti⁴⁺ in metamict zirconolite and titanite: A new occurrence shown by Ti K-edge XANES spectroscopy

FRANÇOIS FARGES

Laboratoire de physique et mécanique des géomatériaux, Université de Marne-la-vallée, URA CNRS 734 and LURE (and Stanford University), 2 rue de la butte verte, 93166 Noisy le Grand cedex, France

ABSTRACT

The coordination environments of Ti in two fully metamict zirconolite samples and two partially metamict titanite samples were determined using high-resolution, X-ray absorption near-edge structure (XANES) spectroscopy at the Ti K edge. Fivefold-coordinated Ti is the dominant Ti species in the zirconolite samples ($\sim 80 \pm 10\%$ of the total Ti atoms). This unusual Ti coordination is also possible in the titanite samples. No significant evidence for ¹⁴⁷Ti was found in any of the samples studied.

Comparison with other amorphous materials, such as other metamict minerals (aeschynite and pyrochlore) and titanosilicate glasses and melts, suggests that fivefold coordination is rather common for Ti⁴⁺ in aperiodic structures. However, the metamict state is characterized by the presence of unusual trigonal bipyramids around ¹⁵¹Ti⁴⁺.