Structure refinement of hydrous andradite, 
\( \text{Ca}_3\text{Fe}_{1.54}\text{Mn}_{0.20}\text{Al}_{0.26}(\text{SiO}_4)_{1.65}(\text{O}_4\text{H}_4)_{1.35} \), from the Wessels mine, Kalahari manganese field, South Africa

THOMAS ARMSTRUSTER

Laboratorium für chemische und mineralogische Kristallographie, Universität Bern, Freiestr. 3, CH-3012 Bern, Switzerland

Abstract: Orange-red, strongly zoned hydrogarnets with octahedral forms occur at the Wessels mine, Kalahari manganese field, South Africa, and are probably of late hydrothermal origin. 'Hydroandradites' from this locality show the highest degree of hydration for andradites hitherto observed in nature.

The crystal structure of such a highly hydrous andradite, \( \text{Ca}_3\text{Fe}_{1.54}\text{Mn}_{0.20}\text{Al}_{0.26}(\text{SiO}_4)_{1.65}(\text{O}_4\text{H}_4)_{1.35} \), \( a = 12.340(1) \) \( \AA \), space group \( \text{Ia}3d \) was refined from single-crystal X-ray data to \( R = 2.38\% \). The structure is composed of disordered micro-domains containing \( \text{SiO}_4 \) and \( (\text{H}_4\text{O}_4) \) tetrahedral units. The distance between \( O \) and the centre of the tetrahedron is \( 1.762(2) \) \( \AA \) representing an average distance between a \( \text{Si}-\text{O} \) bond and a vacancy-\( O \) distance of a \( (\text{H}_4\text{O}_4) \) tetrahedron. Oxygen atoms are strongly smeared out along the \( \text{Si}-\text{O} \) vector caused by a smooth adoption to the local environment. The \( \text{Fe}-\text{O} \) distance of \( 2.021(2) \) \( \AA \) is similar to that in andradite.

Key-words: hydrogarnet, andradite, crystal structure, disorder, Kalahari manganese field.

Introduction

Prominent members of the hydrogarnet family can be derived from grossular (Basso et al., 1983; Passaglia & Rinaldi, 1984; Sacerdoti & Passaglia, 1985) where \( \text{SiO}_4 \) units are partially replaced by \( (\text{H}_4\text{O}_4) \) tetrahedra (e.g. Lager et al., 1987). A hydrogarnet, \( \text{Ca}_3\text{Al}_2(\text{H}_4\text{O}_4)_3 \), without any \( \text{Si} \) can also be synthesized (e.g. Cohen-Addad et al., 1967).

A hydrous component in andradite from the Totalp serpentine (Davos, Switzerland) was discovered by Peters (1965) using powder IR-spectroscopy. Based on a chemical analysis Ford (1970) assumed a hydrous component for andradite from a serpentinite in Tasmania. Since these discoveries many description of hydrous andradites were published (e.g. Onuki et al., 1982; Lager et al., 1989; Armbruster & Geiger, 1993; Müntener & Hermann, 1994). Most of these hydrous andradites are also characterized by octahedral \( \text{Ti} \). If \( \text{Ti} \) is absent, the hydrous component is very low. The term 'hydroandradite' is not an accepted mineral name by the IMA Commission on New Minerals and Mineral Names but it is frequently used in the literature and is stated in the Mineral Database (Aleph Enterprises, 1993).

Von Bezing et al. (1991) and von Bezing & Gutzmer (1994) describe orange-red garnets with octahedral forms from the Wessels mine in the Kalahari manganese field, South Africa. Electron