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Infrared characterization of (OH, F)-pargasites

There has been a great deal of work concerning cation ordering in pargasite in the past ten years. Raudsepp et al. (1987) studied a series of pargasitic amphiboles with different M^{3+} cations at the octahedral strip (Al, Ga, Sc, Cr, In) and showed that in magnesium end-member pargasite there is significant disorder of the trivalent cations over the M(1, 2, 3) octahedra. Single-crystal XRD work (Oberti et al. 1995 a) shows substantial Al occupancy at M(3) in Mg-rich pargasite, in agreement with the data of Raudsepp et al. (1987) and Welch et al. (1994) on synthetic end-member pargasite. Aluminum ordering in pargasite has been recently recognized to be dependent on the octahedral composition of the amphibole: Oberti et al. (1995 a) have shown that the degree of ^[6]Al disorder in natural (Mg, Fe^{2+})-pargasites is inversely related to the amount of Fe^{2+} in the crystal, and Della Ventura et al. (1995) have shown complete ^[6]Al ordering at M(2) in end-member Co-pargasite, suggesting a dominant role of the mean radius of the divalent octahedral cation on the ^[6]Al ordering scheme in the pargasite structure.

Here, we relate the crystal-chemical characterization of pargasites $NaCa_2(Mg_4Al)(Si_6Al_2)O_{22}(OH, F)_2$ along the OH-F substitutional join. The IR spectrum of OH-pargasite (Fig. 1), shows two bands of almost equal intensity which are assigned to the MgMgMg-OH (Aband, at 3710 cm^{-1}) and to the MgMgAl-OH (B-band, at 3678 cm^{-1}) configurations. For increasing F, each of these two bands is replaced by a new band shifted towards lower and constant wavenumbers, whose intensity can be related to the fluorine content of the amphibole: A-band at $3710 \text{ cm}^{-1} \Rightarrow \text{A'-band}$ at 3694 cm^{-1} and B-band at $3678 \text{ cm}^{-1} \Rightarrow \text{B'-band}$ at 3658 cm^{-1} . This twomode behaviour is well known in richterites (Robert et al. 1989) and suggests a vibrational coupling through the cation at the A-site.

The doublet assigned to the MgMgAl-OH configuration (B and B' bands) vanishes, as a function of the fluorine content, more rapidly compared to the one assigned to the MgMgMg environment (A and A' bands) of the OH group. This indicates an increasing ^[6]Al ordering at M(2), for increasing F, in agreement with the XRD data of Oberti et al. (1995 b) which show a complete Al ordering at M(2) in synthetic F-pargasite end-member. The exclusion of Al from the (OH, F)-coordinated M(1, 3)octahedra, for increasing F in the system, may be ex-

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Fig. 1 Evolution of the infrared spectrum of synthetic pargasite, $NaCa_2(Mg_4Al)(Si_6Al_2)O_{22}(OH, F)_2$, along the OH-F substitutional join, as a function of the nominal fluorine content, in atom per formula unit

plained considering the local charge balance around the OH groups bonded to MgMgAl.

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