Linking water contents in mantle pyroxenes and Fe^{3+}

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The incorporation and preservation of hydrogen (water) in nominally anhydrous minerals is of great interest, particularly due to the effects of water on the physical properties of the mantle (e.g. enhances melting, increases electrical conductivity). Although ideally anhydrous, pyroxenes may contain several hundred ppm of water at high pressure and temperature conditions, and are comparatively the most water-rich nominally anhydrous mineral in the mantle. Nevertheless, hydrogen accommodation in the pyroxene structure is still poorly understood.

Previous studies have argued that water as hydroxyl (OH) is preferentially incorporated on the O2 position, with charge compensation given either by cation vacancies in the M2 site, or charge-deficient substitution in the tetrahedral site. Previously, the total water content has been positively correlated with M2 vacancies accompanying Ca-Eskola [1] in clinopyroxene and OH absorbance bands at 3650–3540 cm^{-1} have been related to the amount of Al in the tetrahedral site [2]. The structural accommodation of OH is however challenging, as stoichiometric calculation of the Fe^{3+} content are not reliable and this error further propagates when calculating the amount of Ca-Eskola and Al^{IV}/Al^{VI}. Moreover, pristine mantle pyroxene, free of nano-inclusions of secondary minerals such as sheet silicates are scarce.

This study combines Fe^{3+} quantification via Mossbauer spectroscopy with OH determinations using Fourier Transform Infrared Spectroscopy, applied on pyroxenes from pristine mantle websterites and eclogites. The wide compositional variability along with the lack of contaminants ensure a more reliable dataset and allow the detailed study of the linkage between Fe^{3+} and water incorporation as hydroxyl at mantle conditions.

[1] Skogby *et al.* (2016) *Eur. J. Mineral.***28**, 631-639.
[2] Koch-Müller *et al.* (2004) *Am. Min.* **89**, 921-931