

Investigating fluorine incorporation in nominally anhydrous forsterite (Mg_2SiO_4)

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The bulk of fluorine present in the Earth is believed to be stored in the mantle [1], with much of it locked somewhere within the structures of nominally anhydrous minerals [2]. At such depths, fluorine is harmless to humans. However, when this trapped fluorine reaches the surface via magmatic processes, it can lead to harmful health effects such as fluorosis [3]. Fluorosis results in bones becoming more brittle and prone to fractures due to the excess fluorine in the body. Despite this hazard, fluorine partitioning and incorporation in the mantle are not well understood. Our study uses *ab initio* simulations to unearth where fluorine is preferentially stored in forsterite, the most abundant mineral in the upper mantle. This is accomplished by comparing the reaction enthalpies of different incorporation scenarios in which fluorine atoms may be stored within forsterite. We find that simultaneous substitution of fluorine and hydroxyl (OH^-) in a hydrogarnet-like defect is the easiest way for fluorine to be stored within forsterite. This is likely to do with the inherently similar ionic radii and formal charges between fluoride and hydroxyl ions and also due to the hydrogen bonds helping to stabilize the fluorinated structure. Furthermore, our pressure simulations up to 12 GPa suggest that higher pressures do not improve the favorability of any of the incorporation mechanisms tested. This suggests that there is a vertical heterogeneity in the ability of fluorine to be incorporated into forsterite in the mantle. These results are also being verified by a parallel set of experiments on synthetic forsterite.

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