

## **Cation sites in Al-rich MgSiO<sub>3</sub> perovskites**

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### **ABSTRACT**

Local structure analysis of Al-containing magnesium silicate perovskite has been carried out with X-ray absorption spectra recorded at the Mg, Al, and Si *K*-edges using the SA32 beam-line of SuperAco (Orsay, France). The Al-XAFS spectrum of (MgSi)<sub>0.85</sub>Al<sub>0.3</sub>O<sub>3</sub> perovskite (synthesized in a multi-anvil apparatus) cannot be explained by assuming that Al<sup>3+</sup> occurs in octahedral or dodecahedral sites only. This conclusion is based on comparison between Al-spectrum and those recorded at the Mg and Si *K*-edges for the same structure, general trends found for Al-spectra in various atomic sites, and ab-initio calculations using the FEFF-6 code. Thus, Al appears to be partitioned between both octahedral and dodecahedral perovskite sites. However, the structural accommodations needed to stabilize Al<sup>3+</sup> cation in such different sites are not straightforward. Also, Mg *K*-edge spectra in enstatite and perovskite were compared with those previously reported at the Fe *K*-edge for the same structures, confirming that these two elements are located in the same polyhedra in both structures, and thus that Fe<sup>2+</sup> enters the dodecahedra of the silicate perovskite.