LETTERS Aluminum substitution in MgSiO₃ perovskite: Investigation of multiple mechanisms by ²⁷Al NMR

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ABSTRACT

In the Earth's mantle, the mechanism(s) of solid solution of Al in MgSiO₃ perovskite strongly impacts its thermodynamic and transport properties. We present ²⁷Al NMR data for perovskite samples of nominal composition Mg(Si_{0.9}Al_{0.1})O_{2.95}, to test a mechanism by which Al³⁺ substitutes at the octahedral Si⁴⁺ sites, leaving a corresponding number of O-site vacancies. We find evidence for this process in a significantly greater peak area for Al at B (Si) sites vs. A (Mg) sites in the structure, and the possible identification of a small concentration of five-coordinated Al adjacent to such vacancies. However, substitution of Al³⁺ at the A sites remains significant. As in perovskite-type technological ceramics, O-atom vacancies may play an important role in enhancing ion mobility and the dissolution of water.