## CHEMISTRY AND MINERALOGY OF EARTH'S MANTLE

## The spin state of iron in Fe<sup>3+</sup>-bearing Mg-perovskite and its crystal chemistry at high pressure<sup>†</sup>

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## ABSTRACT

Valence, spin states, and crystallographic sites of Fe in (Mg,Fe)SiO<sub>3</sub> perovskite were investigated using energy-domain <sup>57</sup>Fe-synchrotron Mössbauer spectroscopy and powder X-ray diffraction up to 86 GPa. The volumes of Fe<sup>3+</sup>-bearing perovskite in this study are slightly smaller than those of Mg endmember perovskite. Our Mössbauer data suggest that Fe<sup>3+</sup> prefers A sites coupled with Mg vacancies, which is consistent with previous data at ambient conditions. Fe<sup>3+</sup> in the A site remains in a high-spin state up to 86 GPa, and some fraction of the A site is occupied by Fe<sup>2+</sup> at pressures above 30 GPa. Fe<sup>2+</sup> in the A sites is also in a high-spin state up to 86 GPa. The coupled substitution from Mg<sup>2+</sup> to a highspin state of Fe<sup>3+</sup> and Mg<sup>2+</sup> vacancy would make the volume of perovskite smaller than that of Mg end-member perovskite. If the lower mantle is saturated in silica, perovskite containing high-spin Fe<sup>3+</sup> in A site has a higher density. Such silica oversaturated regions could sink by the density difference.

Keywords: Perovskite, ferric iron, spin state, Mössbauer spectroscopy, X-ray diffraction