

## **High-pressure synthesis of skiagite-majorite garnet and investigation of its crystal structure**

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### **ABSTRACT**

Skiagite-rich garnet was synthesized as single crystals at 9.5 GPa and 1100 °C using a multi-anvil apparatus. The crystal structure [cubic, space group  $Ia\bar{3}d$ ,  $a = 11.7511(2)$  Å,  $V = 1622.69(5)$  Å<sup>3</sup>,  $D_{\text{calc}} = 4.4931$  g/cm<sup>3</sup>] was investigated using single-crystal synchrotron X-ray diffraction. Synchrotron Mössbauer source spectroscopy revealed that Fe<sup>2+</sup> and Fe<sup>3+</sup> predominantly occupy dodecahedral (X) and octahedral (Y) sites, respectively, as expected for the garnet structure, and confirmed independently using nuclear forward scattering. Single-crystal X-ray diffraction suggests the structural formula of the skiagite-rich garnet to be Fe<sub>3</sub><sup>2+</sup>(Fe<sub>0.234(2)</sub><sup>2+</sup>Fe<sub>1.532(1)</sub><sup>3+</sup>Si<sub>0.234(2)</sub><sup>4+</sup>)(SiO<sub>4</sub>)<sub>3</sub>, in agreement with electron microprobe chemical analysis. The formula is consistent with X-ray absorption near-edge structure spectra. The occurrence of Si and Fe<sup>2+</sup> in the octahedral Y-site indicates the synthesized garnet to be a solid solution of end-member skiagite with ~23 mol% of the Fe-majorite end-member Fe<sub>3</sub><sup>2+</sup>(Fe<sup>2+</sup>Si<sup>4+</sup>)(SiO<sub>4</sub>)<sub>3</sub>.

**Keywords:** Skiagite, majorite, garnets, single-crystal X-ray diffraction, Mössbauer spectroscopy, nuclear forward scattering, XANES