

Xuite, $\text{Ca}_3\text{Fe}_2[(\text{Al},\text{Fe})\text{O}_3(\text{OH})]_3$, a new mineral of the garnet group: Implications for the wide occurrence of nanominerals

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ABSTRACT

Xuite, $\text{Ca}_3\text{Fe}_2[(\text{Al},\text{Fe})\text{O}_3(\text{OH})]_3$, is a new member of the garnet supergroup discovered in basaltic scoria from Menan Volcanic Complex, Idaho, U.S.A. Oxidation of Fe-bearing pyroclasts at high temperatures led to the formation of xuite, together with luogufengite, valleyite, and hematite. The measured crystal size of xuite ranges from ~200 to 800 nm. The empirical chemical formula of xuite is $(\text{Ca}_{0.92}\text{Mg}_{0.08})_3(\text{Fe}_{0.96}\text{Ti}_{0.04})_2[(\text{AlO}_4\text{H})_{0.44}(\text{FeO}_4\text{H})_{0.33}(\text{SiO}_4)_{0.05}(\square\text{O}_4\text{H}_4)_{0.18}]_3$. Xuite has a space group of $Ia\bar{3}d$; its unit-cell parameter refined from high-resolution synchrotron X-ray diffraction (XRD) data is $a = 12.5056(5)$ Å, with $Z = 8$ (calculated density = 3.53 g/cm³). Fourier-transform infrared spectroscopy spectrum of xuite shows absorption bands at 3682 and 3579 cm⁻¹, indicating the presence of OH⁻ in the hydrogarnet structure. In situ high-temperature synchrotron XRD combined with thermogravimetry and differential scanning calorimetry reveals that xuite undergoes dehydroxylation to form brownmillerite ($\text{Ca}_2\text{FeAlO}_5$) from ~236 to ~396 °C. Xuite occurs in the form of nanocrystals with a soft magnetic property, which provides important insights into the origin of basaltic scoria and associated paleomagnetism. Xuite was also found in Wyoming paralava, suggesting the possibility of its wide occurrence in various geological environments. The mineral was named after Huifang Xu and Hongwu Xu in honor of their sustained contributions to mineral sciences.

Keywords: Xuite, garnet group, luogufengite, valleyite, synchrotron X-ray diffraction, transmission electron microscopy