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Letter

Chemical composition and crystal structure of merrillite from the Suizhou meteorite

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Abstract

Merrillite, ideally $Ca_9NaMg(PO_4)_7$, is an important accessory phosphate mineral in many different groups of meteorites, including martian meteorites, and a major carrier of rare earth elements (REE) in lunar rocks. By means of electron microprobe analysis, single-crystal X-ray diffraction, and Raman spectroscopy, we present the first structure determination of merrillite with a nearly ideal chemical composition, $Ca_{9.00}Na_{0.98}(Mg_{0.95}Fe_{0.06})_{\Sigma 1.01}(P_{1.00}O_4)_7$, from the Suizhou meteorite, a shock-metamorphosed L6-chondrite. Suizhou merrillite is trigonal with space group $R3c$ and unit-cell parameters a = 10.3444(3), c = 37.0182(11) Å, and V = 3430.5(2) Å^3. Its crystal structure, refined to R_1 = 0.032, is characterized by a structural unit consisting of a $[(Mg,Fe)(PO_4)_6]^{16-}$ complex anion that forms a "bracelet-and-pinwheel" arrangement. Such structural units are linked by interstitial complexes with a formula of $[Ca_9Na(PO_4)]^{16+}$, which differs from that of $[Ca_9(PO_3[OH])]^{16+}$, $[Ca_9(PO_3F)]^{16+}$, $[Ca_9(Ca_{0.5}\square_{0.5})(PO_4)]^{16+}$, or $[(Ca_{9-x}REE)_x(Na_{1-x}\square_x)(PO_4)]^{16+}$ in terrestrial whitlockite, terrestrial/extraterrestrial bobdownsite, meteoritic Ca-rich merrillite, or lunar REE-rich merrillite, respectively. The Suizhou merrillite is found to transform to tuite at high pressures, pointing to the likelihood of finding REE-bearing tuite on the Moon as a result of shock events on REE-merrillite.

Keywords: Merrillite, whitlockite, Suizhou meteorite, crystal structure, Raman spectroscopy