

LETTER

Chemical composition and crystal structure of merrillite from the Suizhou meteorite

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ABSTRACT

Merrillite, ideally $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$, 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, $\text{Ca}_{9.00}\text{Na}_{0.98}(\text{Mg}_{0.95}\text{Fe}_{0.06})_{\Sigma 1.01}(\text{P}_{1.00}\text{O}_4)_7$, 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 $V = 3430.5(2)$ Å³. Its crystal structure, refined to $R_1 = 0.032$, is characterized by a structural unit consisting of a $[(\text{Mg},\text{Fe})(\text{PO}_4)_6]^{16-}$ complex anion that forms a “bracelet-and-pinwheel” arrangement. Such structural units are linked by interstitial complexes with a formula of $[\text{Ca}_9\text{Na}(\text{PO}_4)]^{16+}$, which differs from that of $[\text{Ca}_9(\text{PO}_3[\text{OH}])]^{16+}$, $[\text{Ca}_9(\text{PO}_3\text{F})]^{16+}$, $[\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})(\text{PO}_4)]^{16+}$, or $[(\text{Ca}_{9-x}\text{REE})_x(\text{Na}_{1-x}\square_x)(\text{PO}_4)]^{16+}$ 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