

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 $R\bar{3}c$ 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

INTRODUCTION

Merrillite, ideally $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$, is a primary accessory mineral in many different groups of meteorites, including martian meteorites, and a major storage of rare earth elements (REE) in lunar rocks (e.g., Jolliff et al. 1993; McSween et al. 1996; Xie et al. 2002; Shearer et al. 2015; Adcock et al. 2014). It is considered to be an important phase in exploring the differences in petrogenesis, mantle evolution, and other geologic processes among Earth, Mars, and other planetary bodies (McSween et al. 1996; Shearer et al. 2015 and references therein). Merrillite was originally proposed by Wherry (1917) in honor of George P. Merrill, who first described this mineral from four meteorites (Merrill 1915). However, owing to the chemical and structural similarities between merrillite and terrestrial whitlockite, ideally $\text{Ca}_9\text{Mg}(\text{PO}_4)_6(\text{PO}_3\text{OH})$, there has been a considerable overlap in the use of these two mineral names in the literature. Fuchs (1962) noted the strong resemblances in powder X-ray diffraction data among merrillite, whitlockite, and synthetic $\beta\text{-Ca}_3(\text{PO}_4)_2$, leading him to argue that these three phases were actually the same and the term “merrillite” should be abandoned in favor of “whitlockite.” Subsequent investigations, nevertheless, demonstrated that the structures of merrillite and synthetic $\beta\text{-Ca}_3(\text{PO}_4)_2$ are similar, but not identical to that of terrestrial whitlockite, especially in terms of their lack of an essential hydrogen component that is found in

whitlockite (e.g., Calvo and Gopal 1975; Prewitt and Rothbard 1975; Dowty 1977). Early work on lunar samples also suggested that “lunar whitlockite” is actually more similar in structure to meteoritic merrillite than to terrestrial whitlockite (Fuchs 1971). Thus, Dowty (1977) recommended “merrillite” for the H-free form found in meteorites and “whitlockite” for the terrestrial form. However, because of the lack of definitive structural data for merrillite due to its small crystal size in meteorites, the term “whitlockite” continues to occasionally be used synonymously or interchangeably when describing extraterrestrial merrillite (e.g., Jolliff et al. 1993; McSween et al. 1996; Xie et al. 2002, 2013).

Another confusion about merrillite arises from its chemical variations. In addition to the ideal chemical formula approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA), there are also two other ideal end-members commonly found in meteorites and lunar rocks: a Na-free but Ca-excess form, $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})(\text{Mg},\text{Fe}^{2+})(\text{PO}_4)_7$ and a Na-free but REE-bearing form, $(\text{Ca}_8\text{REE})\square(\text{Mg},\text{Fe}^{2+})(\text{PO}_4)_7$ (e.g., Dowty 1977; Jolliff et al. 1993, 2006; Shearer et al. 2015). These two phases are isostructural with merrillite, but have no official names approved by IMA. To facilitate the following discussion, we will temporarily follow the proposal by Jolliff et al. (2006), whenever it is necessary, by calling the three forms $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$, $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})(\text{Mg},\text{Fe}^{2+})(\text{PO}_4)_7$, and $(\text{Ca}_8\text{REE})\square(\text{Mg},\text{Fe}^{2+})(\text{PO}_4)_7$ as Na-, Ca-, and REE-merrillites, respectively.

Although there have been several structure determinations on

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synthetic or heat-treated merrillites (e.g., Malozov et al. 1997; Hughes et al. 2008; Adcock et al. 2014), the first high-quality single-crystal X-ray structural refinement from a natural sample was only conducted recently by Hughes et al. (2006) using a REE-rich but Na-poor lunar merrillite with the chemistry $(\text{Ca}_{8.42}\text{REE}_{0.69})_{\Sigma 9.11}\text{Na}_{0.20}(\text{Mg}_{0.72}\text{Fe}_{0.31}\text{Mn}_{0.01})_{\Sigma 1.04}(\text{P}_{0.99}\text{O}_4)_7$. Based on this study, Hughes et al. (2006) illustrated the detailed structural differences among lunar merrillite, merrillite reported from meteorites, and terrestrial whitlockite. Jolliff et al. (2006) further suggested that significant structural differences between terrestrial whitlockite and lunar (and meteoritic) varieties warrant the use of “merrillite” for the H-free extraterrestrial material, and the systematic enrichment of REE in lunar merrillite warrants the use of “REE-merrillite.” Yet, there has been no crystal structure report on any, natural or synthetic, Na-rich merrillite to date. This paper presents the first single-crystal X-ray diffraction and Raman spectroscopic study on a natural merrillite with nearly ideal chemistry, $\text{Ca}_{9.00}\text{Na}_{0.98}(\text{Mg}_{0.95}\text{Fe}_{0.06})_{\Sigma 1.01}(\text{P}_{1.00}\text{O}_4)_7$, from the Suizhou meteorite.

The Suizhou meteorite is a shock-metamorphosed L6-chondrite, (Xie et al. 2011). The meteorite contains shock-produced melt veins ranging from 20 to 200 μm in width with a bulk chondritic composition. Major rock-forming minerals in the host meteorite are olivine, pyroxene, plagioclase, kamacite, taenite, and troilite. Accessory minerals include chromite, ilmenite, merrillite, and apatite. Both olivine and pyroxene display moderate mosaic texture, and most of the plagioclase grains were shock-melted and quenched to maskelynite. The shock veins contain abundant high-pressure minerals (e.g., ringwoodite, majorite, akimotoite, vitrified perovskite, lingunite, tuite, xieite, CF-phase, magnesiowüstite, majorite-pyropite garnet solid solution), for which the shock-produced pressure and temperature of 24 GPa and 1900–2000 $^{\circ}\text{C}$ is inferred (Xie et al. 2011).

EXPERIMENTAL METHODS

Merrillite in the Suizhou meteorite makes up about 2 vol% of the chondritic portions (Xie et al. 2002). It occurs as single grains of irregular shape up to 0.5 mm in length (Fig. 1). The grains of merrillite are heavily fractured by shock. The merrillite sample used in this study was selected from a polished section of the shock vein-bearing fragment, which was deposited in the RRUFF Project with the deposition number R150063 (<http://rruff.info/R150063>). Its chemical composition was determined with a Shimadzu 1720 electron microprobe operated at 15 kV and 10 nA with the beam diameter of 1 μm . The standards include albite for Na, MgO for Mg, CaSiO_3 for Ca, Fe_2O_3 for Fe, fluorapatite for P. The average composition (wt%) of 16 analysis points on 10 different grains is CaO 46.76(49), Na_2O 2.82(17), MgO 3.53(15), FeO 0.40(29), and P_2O_5 46.06(43), with a total of 99.62(40), yielding an empirical chemical formula $\text{Ca}_{9.00}\text{Na}_{0.98}(\text{Mg}_{0.95}\text{Fe}_{0.06})_{\Sigma 1.01}(\text{P}_{1.00}\text{O}_4)_7$ on the basis of 28 O atoms, in remarkable agreement with the ideal formula $\text{Ca}_9\text{MgNa}(\text{PO}_4)_7$.

The Raman spectrum of merrillite was collected from a randomly oriented crystal on a Thermo-Almega microRaman system, using a 532 nm solid-state laser with a thermoelectric cooled CCD detector. The laser is partially polarized with 4 cm^{-1} resolution and a spot size of 1 μm .

Single-crystal X-ray diffraction data of merrillite were collected from a nearly equidimensional crystal (0.06 \times 0.07 \times 0.07 mm) on a Bruker X8 APEX2 CCD X-ray diffractometer equipped with graphite-monochromatized $\text{MoK}\alpha$ radiation with frame widths of 0.5 $^{\circ}$ in ω and 30 s counting time per frame. All reflections were indexed on the basis of a hexagonal unit cell (Table 1). The intensity data were corrected for X-ray absorption using the Bruker program SADABS. The systematic absences of reflections suggest possible space group $R3c$ or $R\bar{3}c$. The crystal structure was solved and refined using SHELX97 (Sheldrick 2008) based on space group $R3c$, because it produced the better refinement statistics in terms of bond lengths and angles, atomic displacement parameters, and R factors. The positions of all atoms were refined with the full occupancies and anisotropic displacement parameters. The ratio of Mg vs. Fe at the M site was also refined, yielding Mg = 0.95 and Fe = 0.05, matching that

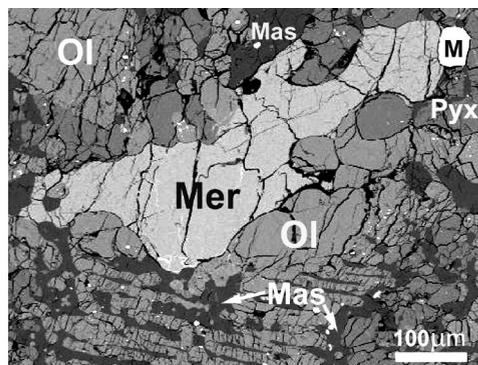


FIGURE 1. Backscattered electron image showing a large merrillite (Mer) grain in the Suizhou meteorite. Ol = olivine, Pyx = Low Ca-pyroxene, Mas = maskelynite, M = FeNi metal.

measured from the chemical composition analysis. Final coordinates and displacement parameters of atoms in merrillite are listed in Table 2, and selected bond distances in Table 3. (CIF¹ available.)

RESULTS AND DISCUSSION

Crystal structure

The crystal structure of merrillite from the Suizhou meteorite is directly comparable with that reported by Hughes et al. (2006) for the REE-rich lunar merrillite. It 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 (Moore 1973) (Fig. 2). The central octahedral cation and the six-coordinating phosphate tetrahedra form a pinwheel, which is characteristic of whitlockite-type compounds. Such structural units are linked by interstitial complexes with a formula of $[\text{Ca}_9\text{Na}(\text{PO}_4)_6]^{16+}$. The major structural difference between the Suizhou merrillite and the lunar REE-rich merrillite is that, due to the coupled substitution of $(\text{REE}^{3+} + \square) \leftrightarrow (\text{Ca}^{2+} + \text{Na}^+)$, the Na site in lunar REE-merrillite is only about 20% occupied, resulting in an average Na-O bond distance (2.71 \AA)

¹Deposit item AM-15-115488, CIF. Deposit items are free to all readers and found on the MSA web site, via the specific issue’s Table of Contents (go to <http://www.minsocam.org/MSA/AmMin/TOC/>).

TABLE 1. Comparison of crystallographic data for various merrillite

	Merrillite	REE-Merrillite	Ca-Merrillite
Sample source	Suizhou meteorite	Apollo 14 lunar rocks	Angra dos Reis achondrite
Ideal chemical formula	$\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$	$(\text{Ca}_8\text{REE})\square(\text{Mg}, \text{Fe}^{2+})(\text{PO}_4)_7$	$\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})_7(\text{Mg}, \text{Fe}^{2+})(\text{PO}_4)_7$
Space group	$R3c$	$R3c$	$R3c$
a (\AA)	10.3444(3)	10.2909(10)	10.362(1)
c (\AA)	37.0182(11)	36.8746(68)	37.106(5)
V (\AA^3)	3430.5(2)	3381.9	3450.3
Z	6	6	6
ρ_{calc} (g/cm^3)	3.121	3.058	3.104
λ (\AA)	0.71073	0.71073	0.7107
μ (mm^{-1})	2.776		2.85
2θ range for data collection	≤ 65.16	≤ 57	
No. of reflections collected	13704	10015	2401
No. of independent reflections	2781	1103	
No. of reflections with $I > 2\sigma(I)$	2279	922	1972
No. of parameters refined	142	147	
$R(\text{int})$	0.046	0.051	
Final R_1 , wR_2 factors [$I > 2\sigma(I)$]	0.032, 0.054	0.045, 0.113	0.041
Final R_1 , wR_2 factors (all data)	0.050, 0.059		
Goodness-of-fit	1.010	1.055	
Reference	This work	Hughes et al. (2006)	Dowty (1977)

TABLE 2. Coordinates and displacement parameters of atoms in merrillite

Atom	x	y	z	U_{eq}	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ca1	0.26876(7)	0.14531(7)	0.67512(2)	0.0138(1)	0.0157(3)	0.0137(3)	0.0130(3)	-0.0026(3)	-0.0012(2)	0.0083(3)
Ca2	0.27190(7)	0.14172(7)	0.56756(1)	0.0121(1)	0.0127(3)	0.0133(3)	0.0107(2)	-0.0009(2)	-0.0002(2)	0.0069(3)
Ca3	0.38354(7)	0.17613(7)	0.76894(1)	0.0122(1)	0.0131(3)	0.0126(3)	0.0103(2)	-0.0002(3)	-0.0013(2)	0.0060(3)
Na	0	0	0.81343(7)	0.0278(6)	0.0267(9)	0.0267(9)	0.0300(16)	0	0	0.0134(5)
M	0	0	-0.00066(5)	0.0108(5)	0.0113(6)	0.0113(6)	0.0100(7)	0	0	0.0056(3)
P1	0	0	0.73382(3)	0.0113(3)	0.0110(4)	0.0110(4)	0.0120(5)	0	0	0.0055(2)
P2	0.31245(9)	0.13793(9)	0.86509(2)	0.0108(2)	0.0107(3)	0.0115(4)	0.0103(3)	0.0007(3)	0.0000(3)	0.0055(3)
P3	0.34393(10)	0.15077(9)	0.96893(2)	0.0104(2)	0.0104(4)	0.0110(4)	0.0096(3)	0.0006(3)	0.0002(3)	0.0051(3)
O1	0	0	0.6928(1)	0.0139(8)	0.0148(12)	0.0148(12)	0.0120(17)	0	0	0.0074(6)
O2	-0.0040(3)	0.1384(2)	0.7475(1)	0.0166(4)	0.0165(10)	0.0137(12)	0.0223(10)	-0.0017(10)	0.0044(8)	0.0094(10)
O3	0.2576(3)	0.0803(3)	0.8265(1)	0.0156(5)	0.0165(11)	0.0171(11)	0.0111(10)	-0.0006(8)	0.0005(9)	0.0067(10)
O4	0.2421(3)	0.2273(3)	0.8792(1)	0.0164(5)	0.0186(12)	0.0202(12)	0.0142(10)	0.0028(9)	0.0038(9)	0.0125(10)
O5	0.2767(2)	-0.0008(2)	0.8880(1)	0.0126(4)	0.0132(10)	0.0119(10)	0.0111(9)	0.0017(8)	0.0009(8)	0.0052(9)
O6	0.4851(2)	0.2392(2)	0.8672(1)	0.0124(4)	0.0117(10)	0.0118(11)	0.0126(9)	0.0008(9)	0.0008(8)	0.0051(10)
O7	0.3784(2)	0.1809(2)	0.0092(1)	0.0127(4)	0.0123(10)	0.0157(11)	0.0092(8)	-0.0007(8)	-0.0022(8)	0.0063(9)
O8	0.3969(3)	0.0427(2)	0.9565(1)	0.0153(5)	0.0162(11)	0.0182(12)	0.0134(10)	-0.0026(9)	-0.0005(9)	0.0102(10)
O9	0.4208(3)	0.2997(3)	0.9488(1)	0.0164(5)	0.0175(11)	0.0143(11)	0.0133(10)	0.0026(9)	0.0003(9)	0.0047(9)
O10	0.1741(2)	0.0767(3)	0.9619(1)	0.0119(4)	0.0101(10)	0.0142(11)	0.0104(9)	-0.0006(9)	-0.0016(8)	0.0053(10)

Notes: The M site is occupied by (0.95 Mg + 0.05 Fe). The labeling scheme of the atomic sites given by Hughes et al. (2006) is adopted here to facilitate a better comparison with the REE-rich merrillite.

TABLE 3. Selected interatomic distances (Å) in the Suizhou merrillite

Ca1-O8	2.386(2)	Ca2-O9	2.313(2)	Ca3-O2	2.363(2)
Ca1-O5	2.413(2)	Ca2-O7	2.361(2)	Ca3-O5	2.373(2)
Ca1-O7	2.472(2)	Ca2-O2	2.450(3)	Ca3-O10	2.418(2)
Ca1-O1	2.497(1)	Ca2-O8	2.467(2)	Ca3-O10	2.431(2)
Ca1-O4	2.517(2)	Ca2-O5	2.477(2)	Ca3-O3	2.436(2)
Ca1-O7	2.531(2)	Ca2-O6	2.479(2)	Ca3-O4	2.443(2)
Ca1-O3	2.626(2)	Ca2-O6	2.489(2)	Ca3-O8	2.634(2)
Ca1-O9	2.628(2)	Ca2-O4	2.833(3)	Ca3-O9	2.689(2)
Avg.	2.509		2.434		2.473
Na-O3	2.411(2) × 3	Mg-O6	2.070(2) × 3		
Na-O2	2.839(3) × 3	Mg-O10	2.089(2) × 3		
Avg.	2.625		2.080		
P1-O1	1.520(4)	P2-O4	1.527(2)	P3-O9	1.529(2)
P1-O2	1.5385(2)	P2-O3	1.541(2)	P3-O7	1.529(2)
P1-O2	1.5385(2)	P2-O5	1.545(2)	P3-O8	1.541(2)
P1-O2	1.539(2)	P2-O6	1.556(2)	P3-O10	1.547(2)
Avg.	1.534		1.542		1.536

slightly longer than that (2.625 Å) in the Suizhou merrillite. According to Hughes et al. (2006, 2008) and Jolliff et al. (2006), the Na site in the interstitial complex unit plays a critical role in maintaining the charge balance in various merrillites. In Ca-merrillite (Calvo and Gopal 1975; Prewitt and Rothbard 1975; Dowty 1977), this site is occupied by (0.5Ca + 0.5□). In other words, it is the configuration and the chemistry of the interstitial complex that defines the differences between whitlockite and merrillite, as well as among Na-, Ca-, and REE-merrillites. The chemical formulas of

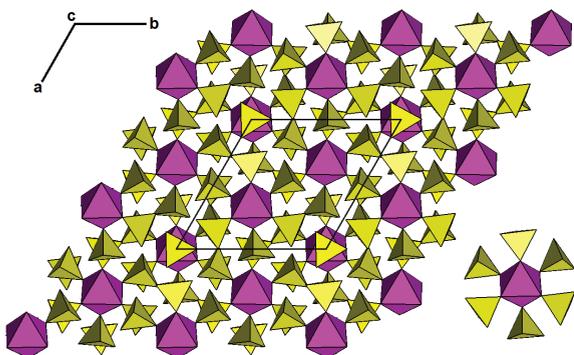


FIGURE 2. The arrangement of the bracelet-and-pinwheel structural units in Suizhou merrillite. A $[(\text{Mg,Fe})(\text{PO}_4)_6]^{16-}$ structure unit is indicated separately at the lower-right corner. (Color online.)

the interstitial complex units are $[\text{Ca}_9(\text{PO}_3[\text{OH}])]^{16-}$, $[\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})(\text{PO}_4)]^{16-}$, and $[(\text{Ca}_{9-x}\text{REE})_x(\text{Na}_{1-x}\square_x)(\text{PO}_4)]^{16-}$ in whitlockite, Ca-merrillite, and REE-merrillite, respectively.

The chief structural difference between merrillite-type and whitlockite-type compounds consists in the configuration of the phosphate tetrahedron in the interstitial complex unit. In whitlockite-type minerals, one of the O^{2-} anions in the phosphate group is substituted by OH^- in whitlockite or F^- in bobdownsite (the F-analog of whitlockite) and the $\text{PO}_3(\text{OH})$ or PO_3F group exhibits an inverted configuration with respect to that in merrillite (e.g., Hughes et al. 2008; Tait et al. 2011). Interestingly, the $\text{PO}_3(\text{OH})$ or PO_3F tetrahedron in natural whitlockite or bobdownsite, respectively, is found to be disordered between the two opposite orientations (with the O-H or P-F bond pointing to either $+\epsilon$ or $-\epsilon$) and the smaller portion of it apparently possesses the same configuration as that in merrillite.

Raman spectroscopy

There have been several investigations on merrillite with Raman spectroscopy and the detailed assignments of major Raman bands have been proposed (e.g., Chen et al. 1995; Jolliff et al. 1996, 2006; Wang et al. 2004). The Raman spectrum of the Suizhou merrillite is displayed in Figure 3, which resembles that of weakly to moderately shocked merrillite in the Sixiangkou meteorite (Chen et al. 1995), merrillite from martian meteorites (Wang et al. 2004), and synthetic REE-poor merrillite (Jolliff et al. 2006). The spectrum of the Suizhou merrillite contains a well-resolved strong doublet at 960 and 976 cm^{-1} , which are attributable to the ν_1 symmetric stretching vibrations of the P-O bonds within the PO_4 tetrahedra. The weak bands between 1018 and 1106 cm^{-1} correspond to ν_3 asymmetric stretching vibrations of the PO_4 groups. The bands ranging from 561 to 524 cm^{-1} are due to the O-P-O bending modes within the PO_4 tetrahedra and those below 479 cm^{-1} to the lattice mode (Jolliff et al. 1996).

The Raman spectrum of the Suizhou merrillite is, however, obviously different from that of the REE-rich merrillite, natural or synthetic, which exhibits an asymmetric single peak or a very poorly resolved doublet (Jolliff et al. 2006). The Raman spectrum of terrestrial whitlockite is similar to that of the REE-rich merrillite, but exhibits an additional weak peak at $\sim 924 \text{ cm}^{-1}$ (Fig. 3) that

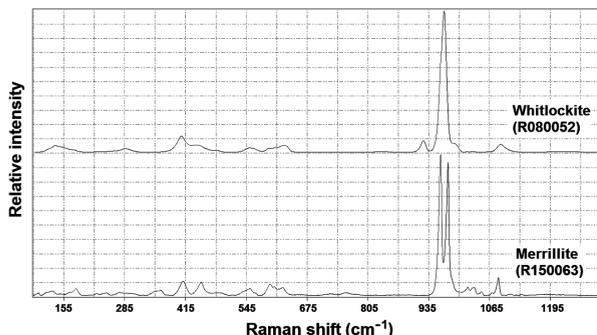


FIGURE 3. Raman spectrum of Suizhou merrillite, along with that of whitlockite for comparison.

is not observed in the spectra of the H-free merrillite. This peak, according to Jolliff et al. (2006), is attributable to the ν_1 symmetric stretching vibrations of the $\text{PO}_3(\text{OH})$ group.

IMPLICATIONS

The Suizhou merrillite has a simple composition with 0.98 Na apfu. This value is much higher than that (0.05–0.20 Na apfu) in lunar merrillites (Hughes et al. 2006; Jolliff et al. 2006), most of which exhibit characteristic enrichment in REE. In comparison, on the one hand, martian merrillite contains significantly higher Na concentrations (up to 0.86 apfu) and much lower REE concentrations (Shearer et al. 2015 and references therein). On the other hand, meteoritic merrillite has relatively low REE contents, but exists in both Ca-rich and Na-rich varieties. Clearly, the simple chemical formula for merrillite, $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$, approved by IMA is insufficient and inadequate to describe various merrillites documented thus far. Accordingly, Jolliff et al. (2006) proposed three merrillite end-member compositions: Ca-merrillite $\text{Ca}_9(\text{Ca}_{0.5}\square_{0.5})\text{Mg}(\text{PO}_4)_7$, Na-merrillite $\text{Ca}_9\text{NaMg}(\text{PO}_4)_7$, and REE-merrillite $[\text{Ca}_8(\text{REE})\square]\text{Mg}(\text{PO}_4)_7$. These merrillite end-members are linked by coupled substitutions: $(0.5\text{Ca}_{\text{Na-site}} + 0.5\square_{\text{Na-site}}) \leftrightarrow \text{Na}_{\text{Na-site}}, \text{Ca}_{\text{Ca-site}} + 0.5\text{Ca}_{\text{Na-site}} \leftrightarrow \text{REE}_{\text{Ca-site}} + 0.5\square_{\text{Na-site}}$, and $0.5\text{Ca}_{\text{Ca-site}} + 0.5\text{Na}_{\text{Na-site}} \leftrightarrow 0.5\text{REE}_{\text{Ca-site}} + 0.5\square_{\text{Na-site}}$. The nomenclature proposed by Jolliff et al. (2006) for various merrillites appears to have its merits, as it reflects their chemical differences and provides considerable conveniences in their descriptions.

Tuite, ideally $\text{Ca}_3(\text{PO}_4)_2$, was first discovered from the Suizhou meteorite as the high-pressure polymorph of merrillite (Xie et al. 2002) or the high-pressure decomposition product of chlorapatite (Xie et al. 2013). It is stable at Earth's mantle temperature-pressure conditions and is proposed to be a potential host for REE and incompatible elements, such as Na, Sr, and Ba (Murayama et al. 1986; Xie et al. 2002). Based on chemical analyses of numerous tuite grains from the Suizhou meteorite, Xie et al. (2013) noticed that tuite converted from merrillite retains similar amounts of MgO and Na_2O as merrillite, whereas that formed through the decomposition of chlorapatite contains little MgO or Na_2O , but significant Cl, suggesting that the Na_2O , MgO, and Cl contents in natural tuite may serve as good indicators for distinguishing its precursor phosphate mineral, merrillite or chlorapatite. It thus begs the question whether REE-bearing tuite could be found on the Moon as a consequence of the REE-merrillite transformation under impacts, as only lunar merrillite exhibits high REE concentrations of all extraterrestrial merrillites documented thus far.

ACKNOWLEDGMENTS

We gratefully acknowledge the funding support from the National Natural Science Foundation of China (Grant No. 41172046 to X.X.) and the Science Foundation Arizona.

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MANUSCRIPT RECEIVED JULY 8, 2015

MANUSCRIPT ACCEPTED AUGUST 10, 2015

MANUSCRIPT HANDLED BY IAN SWAINSON