

**FERROTAFFEITE-2N'2S, A NEW MINERAL SPECIES,
AND THE CRYSTAL STRUCTURE OF Fe²⁺-RICH MAGNESIOTAFFEITE-2N'2S
FROM THE XIANGHUALING TIN-POLYMETALLIC ORE FIELD,
HUNAN PROVINCE, CHINA**

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ABSTRACT

Ferrotaafeite-2N'2S, ideally BeFe₃Al₈O₁₆ with hexagonal symmetry *P6₃mc*, is a new mineral species of the taaffeite group (IMA No. 2011-025) occurring as a skarn mineral in the Xianghualing Sn-polymetallic ore field, Linwu County, Hunan Province, People's Republic of China. It was found near the outer contact of the Laizhiling A-type granite pluton and in the Middle-Upper Devonian carbonate rocks of the Qiziqiao Formation. The associated minerals are Fe²⁺-rich magnesiotaaffeite-2N'2S, ferromagnetite-2N'1S, cassiterite, liberite, pyrite, sphalerite, pyrrhotite, galena, spinel, and phlogopite. The mineral forms tabular crystals about 100 μm in size. It is dark green to dark grey with a white streak, transparent, and has a vitreous lustre. Cleavage is fair on {001}. It is brittle, with a conchoidal fracture. The hardness is VHN₅₀ 1801-2404 kg/mm² (8.5-9 on the Mohs scale). No fluorescence in long- or short-wave ultraviolet radiation was observed. The calculated density from the empirical chemical formula is 3.99 g/cm³. The Gladstone-Dale relationship gives N_{calc} = 1.82. The empirical formula for the investigated ferrotaafeite-2N'2S is Be(Fe_{1.39}Mg_{0.97}Zn_{0.42}Mn_{0.17}Sn_{0.03})_{22.98}Al_{7.99}O₁₆. The simplified formula is Be(Fe,Mg,Zn)₃Al₈O₁₆. The strongest five reflections in the X-ray powder diffraction pattern [*d* in Å (1) *hkl*] are: 2.43(100) 114, 2.60(90) 016, 1.425(90) 220, 2.86(80) 110, and 1.473(80) 0210. The unit-cell parameters refined from the powder data are *a* 5.706(8), *c* 18.352(3) Å, and *V* 517.46(8) Å³, *Z* = 2. The associated Fe²⁺-rich magnesiotaaffeite-2N'2S has empirical formula Be(Mg_{1.54}Fe_{0.98}Zn_{0.38}Mn_{0.14}Sn_{0.02})_{23.06}Al_{7.95}O₁₆. Its structure was solved and refined in space group *P6₃mc*, with *a* 5.6978(8), *b* 5.6978(8), *c* 18.373(4) Å, *V* 516.57(15) Å³, to *R*₁ = 0.043, *wR*₂ = 0.137.

Keywords: ferrotaafeite-2N'2S, new mineral species, magnesiotaaffeite-2N'2S, taaffeite group, Xianghualing tin mine, Tanzanian LM, felsic magmatism, China

INTRODUCTION

According to the IMA-CNMMC nomenclature (Armbruster 2002, Mills *et al.* 2009), minerals of the högbomite, nigerite, and taaffeite groups within the högbomite supergroup form polysomatic series. Minerals of the högbomite and nigerite groups are composed of spinel (*S*) and nolanite (*N*) modules. The idealised formula of a spinel module is *T*₂*M*₄O₈,

where *T* and *M* represent tetrahedrally and octahedrally coordinated cations. The nolanite module has the formula *TM*₄O₇(OH). Minerals of the taaffeite group are composed of spinel (*S*) and modified nolanite (*N'*) modules. The idealised formula of a modified nolanite (*N'*) module is Be*TM*₄O₈, where one additional tetrahedral site is occupied by Be without OH groups. The composition of minerals within the högbomite supergroup depends on: (1) the composition of the *N* or *N'*

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module, (2) the composition of the *S* module, (3) and the number of *S* and *N* or *N'* modules forming the structure. If the molar concentration of $Ti > Sn$, the mineral group is hōgbomite. If the molar concentration of $Sn > Ti$, the mineral group is nigerite. Taaffeite-group minerals have tetrahedral Be but no OH groups.

Taaffeite-group minerals are rare and few localities have been reported (Anderson *et al.* 1951, Nuber & Schmetzer 1983). The taaffeite group consists of three members: magnesiotaaffeite- $2N'2S$ ($a = 5.69$, $c = 18.34$ Å), magnesiotaaffeite- $6N'3S$ ($a = 5.68$, $c = 41.10$ Å), and ferrottaaffeite- $6N'3S$ ($a = 5.70$, $c = 41.16$ Å) (Armbruster 2002, Mills *et al.* 2009).

The crystal structure of magnesiotaaffeite- $2N'2S$ was first described by Peng & Wang (1963) using a sample from Xianghualing, China, assuming the formula $BeMgAl_4O_8$ and $Z = 4$. Nuber & Schmetzer (1983) revised the crystal structure of magnesiotaaffeite- $2N'2S$, investigating a sample from Sri Lanka, and the crystal-chemical formula was given as $BeMg_3Al_8O_{16}$ with $Z = 2$.

In this paper, both Mg-rich ferrottaaffeite- $2N'2S$ and Fe^{2+} -rich magnesiotaaffeite- $2N'2S$ have been examined. Due to the scarcity of single crystals, only the crystal structure of Fe^{2+} -rich magnesiotaaffeite- $2N'2S$ was determined. As an end-member of the taaffeite group, ferrottaaffeite- $2N'2S$ constitutes a new mineral species. The new mineral species and its name have been approved by the Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association (IMA No. 2011-025). The type specimen of ferrottaaffeite- $2N'2S$ is deposited in the collection of the Museum of the Institute of Geology and Geophysics, Chinese Academy of Sciences, Beijing, under specimen number KDX017.

OCCURRENCE OF THE MINERALS

Both Mg-rich ferrottaaffeite- $2N'2S$ and Fe^{2+} -rich magnesiotaaffeite- $2N'2S$ were found at the Xianghualing tin mine in the Xianghualing tin-polymetallic ore field, Linwu County, Chenzhou Prefecture, Hunan Province, People's Republic of China ($112^{\circ}34'E$, $25^{\circ}28'N$). The Xianghualing ore field is geotectonically located at the juncture of the Nanling tectonic zone (extending east-west) and the Leiyang-Linwu tectonic zone (striking north-south). The strata exposed in this area span every age except Ordovician and Silurian. Unconformable Devonian strata lie on a basement of Cambrian slate and meta-sandstone formations, which form the core part of the Xianghualing short-axis anticline. The flank part of the Xianghualing short-axis anticline consists of Middle Devonian glutenite, sandstone and sandy shale of the Tiaomajian Formation, limestone and dolomitic limestone of the Qiziqiao Formation, Upper Devonian dolomitic limestone and sandstone of the Shetianqiao Formation, Carboniferous carbonate, and clastic rock. The Cambrian and Devonian strata are

considered to be the main ore-hosting strata in this ore field (Cai 1991, Luo *et al.* 2010).

The Yanshanian granitoid rocks are prominently developed in this ore field. The Laiziling (2.2 km²) and Jianfengling (4.4 km²) granitic plutons are the principal units, emplaced into the Cambrian-Devonian strata of the Xianghualing short-axis anticline. The intrusive rocks are leucocratic and felsic, and the magma was volatile-enriched (Zhong & Li 2006). The K-Ar ages from biotite for the Laiziling and Jianfengling granite are 155 and 167 My, respectively (Yuan *et al.* 2007), which corresponds to the Late Mesozoic (LM₁) J₂-J₃ episode of post collisional anorogenic magmatism (Zhou *et al.* 2006).

The ore deposits occur around the granite plutons and display obvious zoning in the products of mineralization. The main ore deposit types in this ore field are a granitic Nb-Ta-Sn deposit, a granophyric Sn deposit, a skarn-type Be-Li deposit and wolframite deposit, a W-Sn deposit, a Sn-polymetallic deposit, and a hydrothermal Pb-Zn deposit (Cai 1991).

Ferrottaaffeite- $2N'2S$ and Fe^{2+} -rich magnesiotaaffeite- $2N'2S$ were found near the exocontact zone of the Laiziling granite body and in the Middle-Upper Devonian carbonate rocks of the Qiziqiao Formation. The minerals formed during the skarn stage. Minerals associated them are ferronigerite- $2N'1S$, cassiterite, liberite, pyrite, sphalerite, pyrrhotite, galena, spinel, and phlogopite.

PHYSICAL AND OPTICAL PROPERTIES FOR FERROTAFFEITE- $2N'2S$

Ferrottaaffeite- $2N'2S$ has a tabular form (Fig. 1), whereas the associated Fe^{2+} -rich magnesiotaaffeite- $2N'2S$ occurs as thick hexagonal tabular crystals. The individual grains of ferrottaaffeite- $2N'2S$ attain a size of about 100 μm. As the size of the available ferrottaaffeite- $2N'2S$ crystals is so small, a number of physical and optical properties could not be measured. Ferrottaaffeite- $2N'2S$ is dark green to dark grey with a white streak, transparent, and has a vitreous lustre. Cleavage is fair on {001}. It is brittle, with a conchoidal fracture. The Vickers microhardness is 2107 kg/mm², ranging between 1801 and 2404 kg/mm² (load 50 g), corresponding to 8.5 - 9 on the Mohs hardness scale. No fluorescence in long- or short-wave ultraviolet light was observed. The density calculated from the empirical chemical formula is 3.99 g/cm³ for ferrottaaffeite- $2N'2S$ and 3.90 g/cm³ for Fe^{2+} -rich magnesiotaaffeite- $2N'2S$. The Gladstone-Dale relationship (Mandarino 1981) gives $N_{\text{calc}} = 1.82$ with $Kc = 0.2052$, where $N_{\text{calc}} = D_{\text{calc}}^*$ ($Kc + 1$) for ferrottaaffeite- $2N'2S$.

CHEMICAL COMPOSITION

Chemical analyses were performed using the wavelength-dispersive spectrometry (WDS) mode with

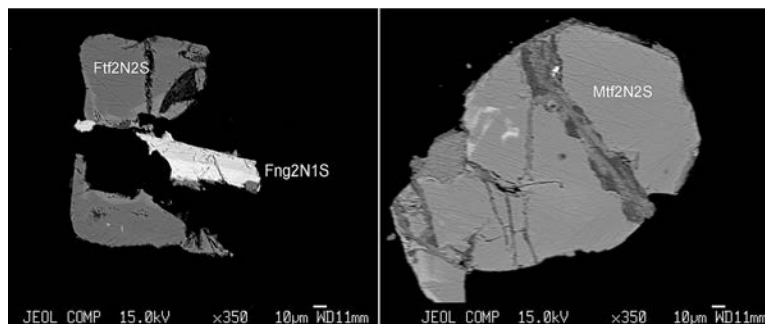


FIG. 1. Back-scattered electron images of ferrotaaffeite-2N'2S (Ftf2N2S), Fe²⁺-rich magnesiotaaffeite-2N'2S (Mtf2N2S) and ferronigerite-2N1S (Fng2N1S) from Xianghualing.

TABLE 1. CHEMICAL COMPOSITIONS OF FERROTAFFEITE-2N'2S (23 ANALYSES) AND Fe²⁺-RICH MAGNESIOTAFFEITE-2N'2S (31 ANALYSES)

Constituent	ferrotaaffeite-2N'2S			Fe ²⁺ -rich magnesiotaaffeite-2N'2S		
	Wt.%	Range	Stand. Dev.	Wt.%	Range	Stand. Dev.
SiO ₂	0.03	0.00-0.35	0.07	0.01	0.00-0.05	0.02
TiO ₂	0.02	0.00-0.08	0.02	0.01	0.00-0.09	0.02
SnO ₂	0.61	0.32-0.85	0.17	0.49	0.24-0.74	0.13
Al ₂ O ₃	66.69	65.75-67.66	0.56	67.16	66.18-68.65	0.74
Cr ₂ O ₃	0.02	0.00-0.08	0.02	0.02	0.00-0.08	0.02
FeO	16.37	13.62-17.48	1.00	11.62	10.72-14.70	0.8
MgO	6.41	5.95-7.31	0.35	10.25	8.32-10.88	0.57
ZnO	5.56	4.42-7.73	0.94	5.06	2.69-7.62	1.64
MnO	1.97	1.57-2.19	0.17	1.67	1.19-2.54	0.48
CaO	0.02	0.00-0.04	0.01	0.01	0.00-0.03	0.01
BaO	0.01	0.00-0.09	0.02	0.02	0.00-0.10	0.02
BeO*	4.09			4.14		
Total	101.80			100.46		
BeO**	3.2			3.1		

*BeO calculated according to stoichiometry

** BeO measured using SIMS.

a JXA-8100 electron-microprobe analyzer. Accelerating voltage and specimen current were maintained at 15 kV and 20 nA. The beam diameter was 2 µm. The following minerals and synthetic materials were used as standards: jadeite for Si and Al, bustamite for Mn and Ca, rutile for Ti, pyrope for Mg, almandine for Fe, SnO₂ for Sn, Cr₂O₃ for Cr, ZnO for Zn, and benitoite for Ba. A Cameca 1280 secondary-ion mass spectrometer (SIMS) was used to measure the content of Be. The single crystal was subjected to bombardment by O ions at 23 keV energy. The beam diameter was 20 µm. Specimen current was maintained at 6.5 nA.

The analytical results for ferrotaaffeite-2N'2S and the associated Fe²⁺-rich magnesiotaaffeite-2N'2S are given in Table 1. The measured amount of Be, using SIMS, is 3.2 wt% BeO for ferrotaaffeite-2N'2S and 3.1 wt% for Fe²⁺-rich magnesiotaaffeite-2N'2S. Because

a Be-bearing glass was used as the standard, in which Be was not distributed evenly, SIMS has a rather poor accuracy. As the refinement does not support any replacement involving Be and Mg, the stoichiometric BeO content, corresponding to 1 atom of Be per formula unit (pfu), was used for calculation.

The average of twenty-three measurements of the full composition of ferrotaaffeite-2N'2S gave the empirical formula Be(Fe_{1.39}Mg_{0.97}Zn_{0.42}Mn_{0.17}Sn_{0.03})_{Σ2.98}Al_{7.99}O₁₆ on the basis of 16 atoms of oxygen and 1 Be *apfu* and assuming that Fe is present as Fe²⁺ and that Mn is present as Mn²⁺. The simplified formula is Be(Fe,Mg,Zn)₃Al₈O₁₆ and the ideal end-member formula is BeFe₃Al₈O₁₆.

The average of thirty-one measurements of the full composition of Fe²⁺-rich magnesiotaaffeite-2N'2S gave the empirical formula Be(Mg_{1.54}Fe_{0.98}Zn_{0.38}M

$n_{0.14}Sn_{0.02}Σ_{3.06}Al_{7.95}O_{16}$. The simplified formula is $Be(Mg,Fe,Zn)_3Al_8O_{16}$ and the ideal end-member formula is $BeMg_3Al_8O_{16}$. The variation of chemical composition of ferrotaafeite-2*N'*2*S* and the associated Fe^{2+} -rich magnesiotaaffeite-2*N'*2*S* are shown in Figure 2.

XRPD DATA FOR FERROTAAFFEITE-2*N'*2*S*

Ferrotaafeite-2*N'*2*S* is hexagonal with space group *P6₃mc*. The X-ray powder diffraction (XRPD) data for ferrotaafeite-2*N'*2*S* were obtained using a Debye-Scherrer camera 114.6 mm in diameter, with $FeK\alpha$ radiation (Table 2). The strongest five reflections in the XRPD pattern (d_{hkl} in Å) are: 2.43₁₁₄ (1 = 100), 2.60₀₁₆ (90), 1.425₂₂₀ (90), 2.86₁₁₀ (80), and 1.473₀₂₁₀ (80). The unit-cell parameters refined from the powder data are *a* 5.706(8), *c* 18.352(3) Å, *V* = 517.46(8) Å³, *Z* = 2. The *c*:*a* ratio calculated from the unit-cell parameters is 3.216. Single-crystal X-ray diffraction studies could not be carried out because of the small size of the crystal and the lack of suitable crystals. However, as larger crystals of the associated Fe^{2+} -rich magnesiotaaffeite-2*N'*2*S* were available, the crystal structure for this mineral was solved.

REFINEMENT OF CRYSTAL STRUCTURE FOR Fe^{2+} -RICH MAGNESIOTAAFFEITE-2*N'*2*S*

Single-crystal X-ray diffraction data for Fe^{2+} -rich magnesiotaaffeite-2*N'*2*S* were collected using

monochromatic $MoK\alpha$ radiation with a Rigaku RA-Micro7HF diffractometer with a Saturn 724+ CCD system. The crystal structure was determined by direct methods (SHELXS-97; Sheldrick 1997) and subsequent Fourier and Fourier difference syntheses. After the determination of all atom positions, the displacement parameters were first refined isotropically, then anisotropically. The refinement procedure was conducted by full-matrix least-square techniques on F^2 .

The structure for Fe^{2+} -rich magnesiotaaffeite-2*N'*2*S* was solved and refined in space group *P6₃mc*, with *a* 5.6978(8), *b* 5.6978(8), *c* 18.373(4) Å, *V* 516.57(15) Å³, to a residual $R_1 = 0.043$ ($wR_2 = 0.137$). The Flack parameter is 0.05(7) and indicates that the structure is not twinned by a center of symmetry operation. According to the crystal-structure refinement, the apparent formula of Fe^{2+} -rich magnesiotaaffeite-2*N'*2*S* is $Be(Mg_{1.73}Fe_{0.89}Zn_{0.32}Sn_{0.06})Σ_3Al_8O_{16}$ with *Z* = 2. Crystal data, data-collection information, and refinement details for Fe^{2+} -rich magnesiotaaffeite-2*N'*2*S* are listed in Table 3. The final coordinates, displacement parameters, and occupancy factors of atoms are given in Table 4. Owing to their similar X-ray scattering power, Mg and Al were not distinguished in the refinement. According to the refinement, the M1, T3, M4, and M5 sites are fully occupied by Al. The final site-occupancy factors (*sof*) for the M2, T6, and T7 sites are constrained according to $Mg + Fe = 1$, $Mg + Fe + Sn = 1$, and $Mg + Zn = 1$, respectively.

The selected interatomic distances are summarized in Table 5. A listing of structure factors and a CIF file

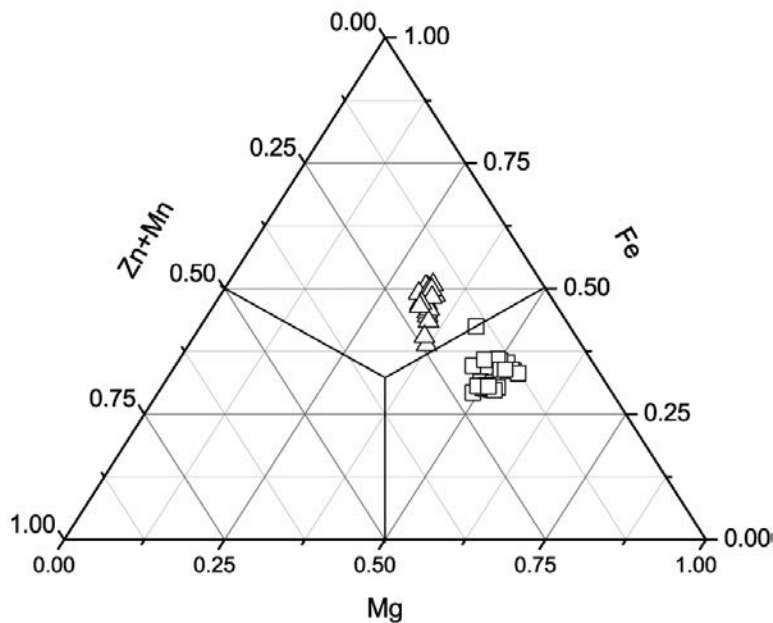


FIG. 2. The variation of chemical compositions for ferrotaafeite-2*N'*2*S* and Fe^{2+} -rich magnesiotaaffeite-2*N'*2*S*.

TABLE 2. POWDER XRD DATA (IN Å) FOR FERROTAFFEITE-2N'2S

<i>l</i>	<i>d</i> _{meas.}	<i>d</i> _{calc.}	<i>h k l</i>	<i>l</i>	<i>d</i> _{meas.}	<i>d</i> _{calc.}	<i>h k l</i>
20	9.2	9.18	0 0 2	40	1.921	1.922	0 2 6
6	4.96	4.94	0 1 0	4	1.889	1.885	0 1 9
6	4.78	4.77	0 1 1	6	1.86	1.858	1 2 1
20	4.56	4.59	0 0 4	6	1.835	1.835	0 0 10
20	4.35	4.35	0 1 2	4	1.8	1.798	0 2 7
10	3.85	3.84	0 1 3	10	1.732	1.73	1 2 4
50	3.36	3.36	0 1 4	10	1.72	1.72	0 1 10
4	3.04	3.06	0 0 6	20	1.682	1.681	0 2 8
60	2.95	2.95	0 1 5	20	1.665	1.665	1 2 5
80	2.86	2.85	1 1 0	20	1.65	1.647	0 3 0
10	2.73	2.72	1 1 2	4	1.645	1.641	0 3 1
90	2.6	2.6	0 1 6	70	1.595	1.59	0 3 3
20	2.45	2.45	0 2 1	30	1.575	1.573	0 2 9
100	2.43	2.42	1 1 4	50	1.551	1.55	0 3 4
60	2.39	2.39	0 2 2	30	1.54	1.543	1 1 10
20	2.32	2.32	0 1 7	10	1.505	1.503	0 3 5
10	2.29	2.29	0 0 8	80	1.473	1.473	0 2 10
40	2.18	2.18	0 2 4	90	1.425	1.426	2 2 0
4	2.08	2.08	0 1 8	40	1.383	1.383	0 2 11
70	2.05	2.05	0 2 5				

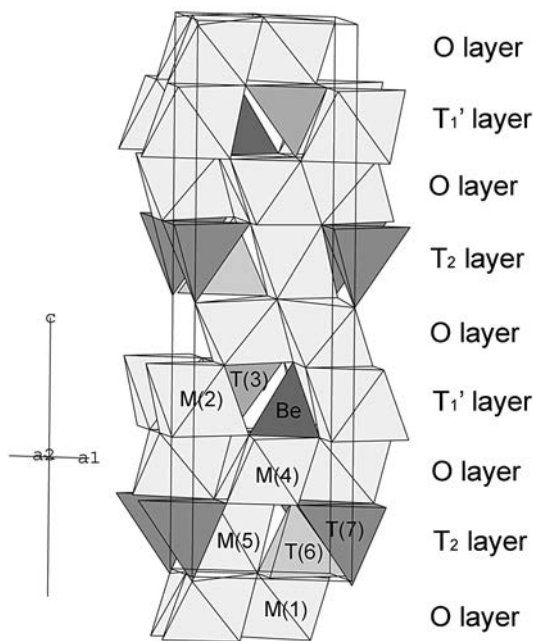


FIG. 3. Polyhedral representation of the Fe²⁺-rich magnesiotaaffeite-2N'2S structure with unit-cell outlines. Light grey octahedra = M5O₆, M2O₆, M4O₆ and M1O₆; light grey tetrahedron = T6O₄; grey tetrahedron = T3O₄; dark grey tetrahedron = T7O₄; dark tetrahedron = BeO₄.

are available from the Depository of Unpublished Data on the Mineralogical Association of Canada website [document Magnesiotaaffeite-2N'2S CM50_21].

DESCRIPTION OF CRYSTAL STRUCTURE FOR Fe²⁺-RICH MAGNESIOTAFFEITE-2N'2S

In general, the structures of minerals within the hōgbomite supergroup are based on a closed-packed oxygen framework with three types of cation layers (Nuber and Schmetzer 1983, Hejny *et al.* 2002). In the case of minerals of the hōgbomite and nigerite groups, these cation layers are:

O layers with three metal atoms per layer in the unit-cell in octahedral sites,

T₁ layers with one metal atom in octahedral and one metal atom in tetrahedral sites,

T₂ layers with one metal atom in octahedral and two metal atoms in tetrahedral sites.

In the case of minerals of taaffeite group, besides **O** layers and **T₂** layers, **T₁** layers are modified into **T₁'** layers with one metal atom in an octahedral site and one Be and one metal atom in tetrahedral sites.

In the case of Fe²⁺-rich magnesiotaaffeite-2N'2S, these cation layers are (Table 4, Fig. 3):

O layers with M(1) or M(4) in octahedral sites,
T₁' layers with M(2) in octahedral, T(3) and Be in tetrahedral sites,

T₂ layers with M(5) in octahedral, T(6) and T(7) in tetrahedral sites.

The cation-layer sequence in Fe²⁺-rich magnesiotaaffeite-2N'2S can be described as **O-T₂-O-T₁'-O-T₂-O-T₁'**, where **O-T₂** represents a spinel

module (*S*) and **O-T₁'** represents a modified nolanite (*N'*) module (Figs. 3-6). The framework of Fe²⁺-rich magnesiotaaffeite-2*N'*2*S* is composed of two spinel modules (*S*) and two modified nolanite modules (*N'*), yielding the sequence *SN'SN'*. Because the idealised

formula of a spinel module and a modified nolanite (*N'*) module are *T₂M₄O₈* and *BeTM₄O₈*, respectively, an idealised taaffeite-2*N'*2*S* polysome has the composition $2 \times (\text{BeT}_3\text{M}_8\text{O}_{16})$.

The crystal structure of Fe²⁺-rich magnesiotaaffeite-2*N'*2*S* from Xianghualing is similar to that from Sri Lanka, and related to ferrohögbohmite-2*N*2*S*. Cation assignment for Fe²⁺-rich magnesiotaaffeite-2*N'*2*S* can be compared with those of magnesiotaaffeite-2*N'*2*S* studied by Peng & Wang (1963), magnesiotaaffeite-2*N'*2*S* by Nuber & Schmetzer (1983), and ferrohögbohmite-2*N*2*S* (3) by Hejny *et al.* (2002), as shown in Table 6. It indicates that the replacements of Mg and Fe were found at the M2, T6, and T7 sites in Fe²⁺-rich magnesiotaaffeite-2*N'*2*S*, while no replacement of cations was found in the crystal structures determined by Peng & Wang (1963) and by Nuber & Schmetzer (1983).

The average M-O distances (M1-O, M2-O, M4-O, M5-O) in Fe²⁺-rich magnesiotaaffeite-2*N'*2*S* range from 1.911 to 2.117 Å and, similar to those, from 1.907 to 2.110 Å [Al3-O, Mg1-O, Al2-O, Al4-O] in magnesiotaaffeite-2*N'*2*S* studied by Nuber & Schmetzer (1983). T3 has a smaller cation-oxygen distance of 1.785 Å than T6 (1.933 Å) and T7 (1.947 Å) in Fe²⁺-rich magnesiotaaffeite-2*N'*2*S*. The corresponding cation-oxygen distances are 1.790 Å (Al1-O), 1.912 Å (Mg3-O), and 1.944 Å (Mg2-O) in magnesiotaaffeite-2*N'*2*S*. In both cases T3 was fully occupied by Al.

CONCLUSIONS

Ferrotaaaffeite-2*N'*2*S* is the Fe²⁺ analogue of magnesiotaaffeite-2*N'*2*S*, *BeMg₃Al₈O₁₆* (Nuber & Schmetzer

TABLE 3. CRYSTAL DATA, DATA COLLECTION INFORMATION AND REFINEMENT DETAILS FOR FE²⁺-RICH MAGNESIOTAFFEITE-2*N'*2*S*

Refined formula	Be(Mg,Fe,Zn,Sn) ₃ Al ₈ O ₁₆
Formula weight	606.43
Space group	<i>P</i> 6 ₃ <i>mc</i>
<i>a</i> (Å)	5.6978(8)
<i>b</i> (Å)	5.6978(8)
<i>c</i> (Å)	18.373(4)
γ (°)	120
<i>V</i> (Å ³), <i>Z</i>	516.57(15), 2
μ (mm ⁻¹)	3.278
Crystal dimensions (mm)	0.40 × 0.27 × 0.15
<i>F</i> (000), ρ _{calc} (cm ⁻³)	590, 3.899
Diffractometer	Saturn 724+ CCD system
λ (MoKα)(Å), T(K)	0.71073, 293(2)
θ range for collection (°)	2.22 to 30.49
<i>h</i> , <i>k</i> , <i>l</i> ranges	-6→8, -8→7, -26→26
Total reflections measured	5022
Unique reflections	672 [R(int) = 4.59%]
Reflections > 4Σ(<i>F</i>)	668
Refinement on	<i>F</i> ²
<i>R</i> ₁ (<i>F</i>), <i>wR</i> ₂ (<i>F</i> ²)	4.27%, 13.74%
<i>R</i> _{1all} (<i>F</i>), <i>wR</i> _{2all} (<i>F</i> ²)	4.41%, 14.94%
Extinct. Coefficient	0.00(4)
No. of refined parameters	74
Goof on <i>F</i> ²	1.019
Δρ _{min} , Δρ _{max} (e/Å ³)	-0.993, 0.987

TABLE 4. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS (IN Å²) WITH E.S.D.'S IN PARENTHESES FOR FE²⁺-RICH MAGNESIOTAFFEITE-2*N'*2*S*

Layer	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	<i>U</i> _{eq}	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₂₃	<i>U</i> ₁₃	<i>U</i> ₁₂	
M1	O	0.6674(4)	0.83369(19)	0.94034(11)	0.0106(5)	0.0095(8)	0.0105(7)	0.0114(9)	0.0003(3)	0.0005(7)	0.0047(4)
M2	T₁'	0	0	0.8008(2)	0.0154(5)	0.0150(7)	0.0150(7)	0.0164(9)	0	0	0.0075(3)
T3	T₁'	0.6667	0.3333	0.8507(3)	0.0084(7)	0.0103(9)	0.0103(9)	0.0048(16)	0	0	0.0051(5)
Be	T₁'	0.3333	-0.3333	0.7940(11)	0.014(3)	0.014(4)	0.014(4)	0.012(9)	0	0	0.007(2)
M4	O	0.0015(4)	0.5008(2)	0.69539(14)	0.0100(4)	0.0094(8)	0.0097(6)	0.0110(9)	0.0003(3)	0.0007(6)	0.0047(4)
M5	T₂	0.6667	0.3333	0.5689(3)	0.0102(8)	0.0097(9)	0.0097(9)	0.011(2)	0	0	0.0048(5)
T6	T₂	0.3333	-0.3333	0.53471(13)	0.0076(7)	0.0083(8)	0.0083(8)	0.0060(14)	0	0	0.0042(4)
T7	T₂	0	0	0.59987(19)	0.0071(5)	0.0080(6)	0.0080(6)	0.0052(9)	0	0	0.0040(3)
O1		0	0	0.9916(6)	0.0136(19)	0.010(2)	0.010(2)	0.021(5)	0	0	0.0050(11)
O2		0.0396(10)	0.5198(5)	0.0023(3)	0.0136(10)	0.018(2)	0.0111(14)	0.014(2)	-0.0021(9)	-0.0042(18)	0.0092(12)
O3		0.3333	-0.3333	0.8864(4)	0.0136(16)	0.020(2)	0.020(2)	0.000(3)	0	0	0.0102(12)
O4		0.8374(5)	0.6748(11)	0.8830(2)	0.0113(9)	0.0139(15)	0.014(2)	0.0061(17)	-0.0016(14)	-0.0008(7)	0.0070(10)
O5		-0.3333	-0.6667	0.7540(4)	0.0058(16)	0.006(2)	0.006(2)	0.005(4)	0	0	0.0032(10)
O6		0.6274(9)	0.8137(5)	0.7541(2)	0.0107(9)	0.013(2)	0.0098(14)	0.0106(19)	0.0010(8)	0.0019(16)	0.0064(10)
O7		0.3333	0.6667	0.6396(5)	0.0120(18)	0.014(2)	0.014(2)	0.009(3)	0	0	0.0068(12)
O8		0.8162(5)	0.6324(9)	0.6361(2)	0.0107(9)	0.0125(16)	0.017(2)	0.0042(17)	0.0002(17)	0.0001(8)	0.0085(10)

Occupancy: M1 = 1.0Al; M2 = 0.597(4)Fe + 0.403(4)Mg; T3 = 1.0Al; M4 = 1.0Al; M5 = 1.0Al; T6 = 0.649(4)Mg + 0.288(10)Fe + 0.063(8)Sn; T7 = 0.678(4)Mg + 0.322(4)Zn.

FIG. 4. Polyhedral representations of the O-layers in the Fe²⁺-rich magnesiotaaffeite-2N'2S structure seen along c. Light grey octahedron = M(4)O₆.

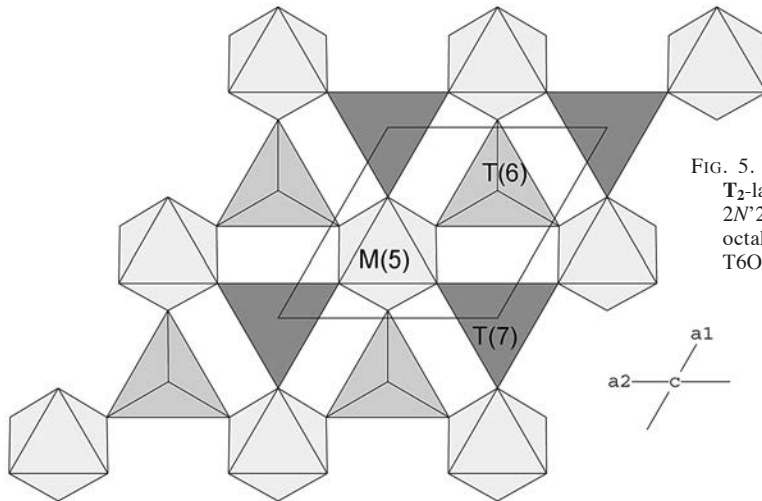
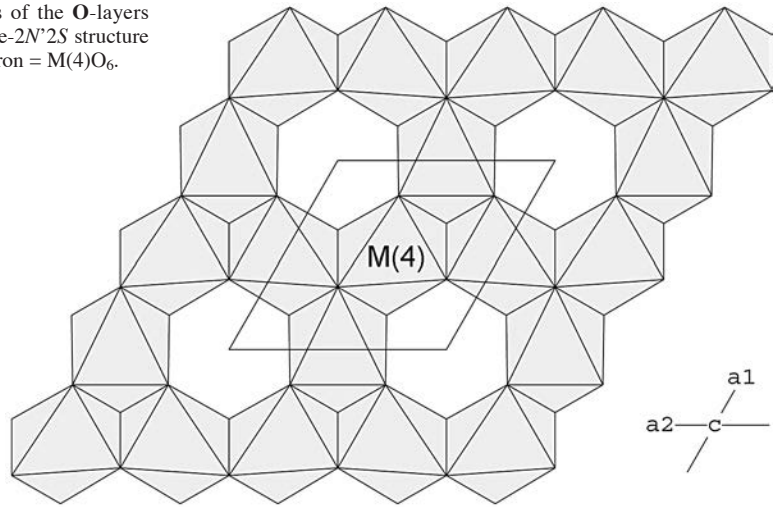
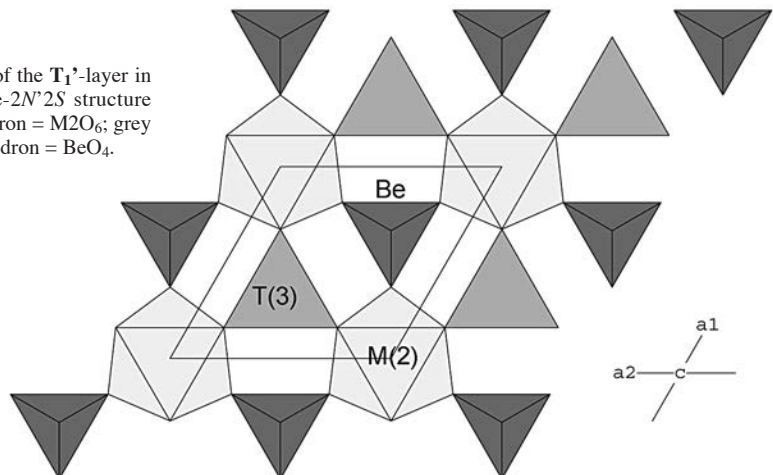


FIG. 5. Polyhedral representation of the T₂-layer in the Fe²⁺-rich magnesiotaaffeite-2N'2S structure seen along c. Light grey octahedron = M5O₆; grey tetrahedron = T6O₄; dark grey tetrahedron = T7O₄.

FIG. 6. Polyhedral representation of the T₁'-layer in the Fe²⁺-rich magnesiotaaffeite-2N'2S structure seen along c. Light grey octahedron = M2O₆; grey tetrahedron = T3O₄; dark tetrahedron = BeO₄.



1983), and is a new end-member of the taaffeite group (new Dana group 07.02.11) within the hōgbomite supergroup (Armbruster 2002, Mills *et al.* 2009). Comparison of the new end member ferrotaafeite-2N'2S with the intermediate Fe²⁺-rich magnesiotaaffeite-2N'2S and end-member magnesiotaaffeite-2N'2S is known in (Table 7).

The refinement of the crystal structure for the Fe²⁺-rich magnesiotaaffeite-2N'2S led to the ideal formula BeMg₃Al₈O₁₆ with Z = 2. No evidence of replacement of Be and Mg in the structure of magnesiotaaffeite-2N'2S was found in this refinement. This is in agree-

ment with result of Nuber & Schmetzer (1983) and further discard the formula Be₂Mg₂Al₈O₁₆ with Z = 4 by Peng & Wang (1963).

ACKNOWLEDGEMENTS

The authors acknowledge the help of Dr. Qiuli Li with the SIMS analyses and Dr. Xiang Hao in the collection of single-crystal structure data at the Institute of Chemistry, Chinese Academy of Sciences. The project was supported by the National Natural Science Foundation of China (No. 40872044). We also wish to thank the referees and associate editor for their insightful input.

TABLE 5. SELECTED INTERATOMIC DISTANCES (Å) FOR THE COORDINATION POLYHEDRA IN FE²⁺-RICH MAGNESIOTAFFEITE-2N'2S

M1O ₆		M4O ₆	
M1-O1	1.892(6)	M4-O7	1.931(6)
-O2 ×2	1.929(4)	-O6 ×2	1.891(3)
-O4 ×2	1.935(3)	-O8 ×2	1.912(3)
-O3	1.923(5)	-O5	1.972(5)
<M1-O> ₆	1.924	<M4-O> ₆	1.918
M2O ₆		M5O ₆	
M2-O6 ×3	2.029(5)	M5-O2 ×3	1.897(6)
-O4 ×3	2.204(6)	-O8 ×3	1.924(6)
<M2-O> ₆	2.117	<M5-O> ₆	1.911
T6O ₄		T7O ₄	
T6-O7	1.928(10)	T7-O1	1.990(12)
-O2 ×3	1.934(5)	-O8 ×3	1.932(5)
<T6-O>	1.933	<T7-O>	1.947
T3O ₄		BeO ₄	
T3-O5	1.777(8)	Be-O3	1.70(2)
-O4 ×3	1.787(5)	-O6 ×3	1.625(10)
<T3-O>	1.785	<Be-O>	1.644

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TABLE 6. CATION ASSIGNMENT FOR FE²⁺-RICH MAGNESIOTAFFEITE-2N'2S (THIS STUDY), MAGNESIOTAFFEITE-2N'2S (1) (PENG & WANG 1963), MAGNESIOTAFFEITE-2N'2S (2) (NUBER & SCHMETZER 1983), AND FERROHÖGBOMITE-2N2S (3) (HEJNY *ET AL.* 2002)

	Layer	This study	1	2	Layer	3
M1	O	Al	Al	Al	O	Al
M2	T ₁ '	(Fe,Zn) _{0.60} Mg _{0.40}	Al	Mg	T ₁	Fe _{0.60} Ti _{0.40}
T3	T ₁ '	Al	Mg	Al	T ₁	(Al,Mg) _{0.57} (Fe,Zn) _{0.43}
Be	T ₁ '	Be	Be	Be	T ₁	H
M4	O	Al	Al	Al	O	Al
M5	T ₂	Al	Al	Al	T ₂	Al
T6	T ₂	Mg _{0.65} (Fe,Zn,Sn) _{0.35}	Mg	Mg	T ₂	(Fe,Zn) _{0.89} (Mg,Al) _{0.11}
T7	T ₂	Mg _{0.68} (Fe,Zn) _{0.32}	Be	Mg	T ₂	(Fe,Zn) _{0.68} (Mg,Al) _{0.32}

Fe²⁺-rich magnesiotaaffeite-2N'2S (this study)

Refined formula: Be(Mg_{1.73}Fe_{0.89}Zn_{0.32}Sn_{0.06})_{Σ3.00}Al₈O₁₆

Analyzed composition: Be(Mg_{1.54}Fe_{0.98}Zn_{0.38}Mn_{0.14}Sn_{0.02})_{Σ3.06}Al_{7.95}O₁₆.

Magnesiotaaffeite-2N'2S (1) (Peng & Wang 1963)

Refined formula: Be₂Mg₂Al₈O₁₆.

Magnesiotaaffeite-2N'2S (2) (Nuber & Schmetzer 1983)

Refined formula: BeMg₃Al₈O₁₆

Analyzed composition: Be(Mg_{2.81}Fe_{0.15}Zn_{0.04})_{Σ3.00}Al₈O₁₆.

TABLE 7. COMPARISON OF UNIT CELL PARAMETERS FOR (1) FERROTAAFFEITE-2N'2S, (2) Fe²⁺-RICH MAGNESIOTAAFFEITE-2N'2S, AND (3) MAGNESIOTAAFFEITE-2N'2S

	1	2	3*
Formula	Be(Fe _{1.39} Mg _{0.97} Zn _{0.42} Mn _{0.17} Sn _{0.03}) _{Σ2.98} Al ₈ O ₁₆	Be(Mg _{1.54} Fe _{0.98} Zn _{0.38} Mn _{0.14} Sn _{0.02}) _{Σ3.06} Al ₈ O ₁₆	Be(Mg _{2.81} Fe _{0.15} Zn _{0.04}) _{Σ3} Al ₈ O ₁₆
Space group	<i>P</i> 6 ₃ <i>mc</i>	<i>P</i> 6 ₃ <i>mc</i>	<i>P</i> 6 ₃ <i>mc</i>
a (Å)	5.706(8)	5.6978(8)	5.6867(6)
c (Å)	18.352(3)	18.373(4)	18.337(3)
V (Å ³)	517.46(8)	516.57(15)	513.54(6)
Z	2	2	2
Density (calc.) (g/cm ³)	3.99	3.90	3.62

* Nuber & Schmetzer 1983

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Received November 28, 2011, revised manuscript accepted March 4, 2011.