# Magnesiosadanagaite, a new member of the amphibole group from Kasuga-mura, Gifu Prefecture, central Japan

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Abstract: Magnesiosadanagaite, ideally NaCa<sub>2</sub>[Mg<sub>3</sub>(Al, Fe<sup>3+</sup>)<sub>2</sub>]Si<sub>5</sub>Al<sub>3</sub>O<sub>22</sub>(OH)<sub>2</sub>, is a new member of the amphibole group occurring as rims of zoned amphibole in rock samples from the contact aureole in Kasuga-mura, central Japan. The amphibole is associated with phlogopite, titanite, calcite, pyrrhotite and chalcopyrite, and composed of an <sup>[4]</sup>Al-poorer core and <sup>[4]</sup>Al-richer rim. The core and rim are classified into pargasite [<sup>[4]</sup>Al = 1.84-2.19 atoms per formula unit (apfu); for O = 23] and pargasite-magnesiosadanagaite (<sup>[4]</sup>Al = 2.45-2.84 apfu), respectively. Both have relatively high <sup>[A]</sup>Na (0.67-0.96 apfu) and low K content (< 0.29 apfu). The high <sup>[A]</sup>Na (0.70-0.92 apfu) and low K (0.09-0.28 apfu) values of magnesiosadanagaite refute the view that high K substitution at the A site is an essential feature of Si-poor calcic amphiboles. The crystal structure of magnesiosadanagaite was refined for two compositionally different samples. Magnesiosadanagaite has the lowest O(5)-O(6)-O(5) angles (160.4° and 161.8°) ever reported in *C2/m* amphiboles, indicating maximal kinking of the double-chain of tetrahedra.

Key-words: magnesiosadanagaite, new mineral species, Si-poor amphibole, structure refinement, Japan.

# Introduction

The silica-poor [Si < 5.5 atoms per formula unit (apfu) for O = 23] calcic amphibole sadanagaite and its Mg-rich analogue, magnesiosadanagaite, were both first identified and described by Shimazaki et al. (1984) from skarns of the amphibolite facies in the Ryoke metamorphic belt. Their ideal chemical formulae were defined as (K,Na)Ca2 (Fe<sup>2+</sup>,Mg,Al,Fe<sup>3+</sup>,Ti)<sub>5</sub>(Si,Al)<sub>8</sub>O<sub>22</sub>(OH)<sub>2</sub> for sadanagaite and (K,Na)Ca<sub>2</sub>(Mg,Fe<sup>2+</sup>,Al,Fe<sup>3+</sup>,Ti)<sub>5</sub>(Si,Al)<sub>8</sub>O<sub>22</sub>(OH)<sub>2</sub> for magnesiosadanagaite. Sadanagaite was also found from skarns in Cornwall (van Marcke de Lumen & Verkaeren, 1985), thermally metamorphosed rocks in the Nogo-Hakusan area (Sawaki, 1989) and Caledonian metamorphic rocks in the Western Baikal region (Savel'eva & Korikovskii, 1998). Magnesiosadanagaite was also reported from metabasites and metacarbonates in the Eastern Alps (Mogessie et al., 1986) and a ruby deposit in China (Wang et al., 1997). These amphiboles, except for those from the Eastern Alps and China, characteristically show a high K<sub>2</sub>O content (K = 0.43-0.84 apfu). Recently, amphibole nomenclature was revised by the Amphibole Subcommittee of the

International Mineralogical Association Commission on the New Minerals and Mineral Names (CNMMN) (Leake et al., 1997). According to the current nomenclature, sadanagaite and magnesiosadanagaite are defined as [A]Na (Na in the A site)-dominant and Si-poor (< 5.5 apfu) calcic amphiboles, ideally NaCa<sub>2</sub>[Fe<sub>3</sub><sup>2+</sup>(Al,Fe<sup>3+</sup>)<sub>2</sub>]Si<sub>5</sub>Al<sub>3</sub>O<sub>22</sub>(OH)<sub>2</sub> and NaCa<sub>2</sub>[Mg<sub>3</sub>(Al,Fe<sup>3+</sup>)<sub>2</sub>]Si<sub>5</sub>Al<sub>3</sub>O<sub>22</sub>(OH)<sub>2</sub>, respectively. Moreover this nomenclature scheme defines prefixes (e.g., fluoro, potassic) that are an essential part of an amphibole name. The prefix "potassic" is related to K > 0.5 apfu and applies to all amphibole groups (Leake et al., 1997). According to this new definition, "sadanagaite" and "magnesiosadanagaite", which were once approved by CNMMN (Nos. 80-27 and 82-102) and reported by Shimazaki et al. (1984), have been redefined into potassicsadanagaite and potassic-magnesiosadanagaite, respectively because they are potassium-dominant-species. The amphiboles described initially as sadanagaite in the literature are potassicsadanagaite except for those from Cornwall (van Marcke de Lumen & Verkaeren, 1985), whereas the amphiboles reported initially as magnesiosadanagaite (e.g., Mogessie et al., 1986; Wang et al., 1997) possess more

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after Suzuki (1977), showing the sample localities.

<sup>[A]</sup>Na than K except for those described by Shimazaki *et al.* (1984). However, the <sup>[A]</sup>Na-rich members, sadanagaite and magnesiosadanagaite have not been formally described as a species until now. Recently, potassic-ferrisadanagaite was described as a new species from an alkaline complex in the Ilmen Mountains (Sokolova *et al.*, 2000).

The amphibole, which has chemical and structural properties that conform to the new nomenclature of magnesiosadanagaite (Leake *et al.*, 1997), was found in a granitic contact aureole in Kasuga-mura, Gifu Prefecture, central Japan. The mineral data and mineral name have been approved by CNMMN (No. 2002-051). In this paper, we will present the mode of the occurrence, chemistry and crystallographic data for magnesiosadanagaite from this locality. The type specimens of magnesiosadanagaite are deposited at the Geological Museum, Geological Survey of Japan, AIST, Tsukuba under the registered number GSJ M35151 and National Science Museum, Tokyo under the catalogue No. NSM-M28307.

## Geological setting and petrography

The Kasuga-mura area comprises the Jurassic formation and Cretaceous Kaizuki-yama granite. The Jurassic formation consists of shale, sandstone and chert with a substantial amount of basic volcanic rocks, dolomite and limestone. The formation was thermally metamorphosed by the Kaizuki-yama granite. The contact aureole around the Kaizuki-yama granite was recognized with a width of more than 3 km. Its metamorphic grade ranges from the greenschist to amphibolite facies (Suzuki, 1975, 1977). Metamorphic zoning is shown in Fig. 1 after Suzuki (1977). The contact aureole is divided into four zones on the basis of mineral parageneses in siliceous dolomite; zone 1 is defined by the presence of talc, zone 2 by the dolomite-quartz-tremolite-calcite assemblage, zone 3 by the diopside-dolomite assemblage and zone 4 by the forsterite-diopside assemblage. Magnesiosadanagaite from three samples, sample numbers GSJ M35151-1, M35151-2 and M35151-3, was examined. The sample GSJ M35151-1 was collected from dump material in the Kasuga mine's Kawai pit, which had produced wollastonite and dolomite. Two other samples GSJ M35151-2 and M35151-3 were collected from basic nodules (up to about 1.5 m in length and 0.5 m in width), which locally occur in dolomitecalcite marble in zone 4 (Fig. 1). The dolomite-calcite marble commonly contains skarn minerals such as grossular, diopside and wollastonite.

All rock samples contain amphibole, phlogopite, titanite, calcite, pyrrhotite and chalcopyrite. Sample GSJ M35151-1 also contains scapolite and apatite with minor amounts of chlorite and pyrite. The other two samples contain minor spinel, pentlandite, ilmenite, apatite (only in GSJ M35151-2), and chlorite (only in GSJ M35151-3).

The amphibole occurs as prismatic crystals, up to 3 mm in length. Most amphibole crystals exhibit distinct optical zoning (Fig. 2). The rim is characterized by stronger pleochroism (yellowish brown to pale yellowish brown) than the core (pale greenish brown to pale brown). In some cases, the zoning is not concentric, and a part of the core contacts directly with the matrix. The boundary between the core and rim is sharp, and the rim has higher refractive indices than the core.

Phlogopite is pale brown and occurs as plates about 0.1-1 mm in length or aggregates of finer crystals (20-30  $\mu$ m). The latter occurrence was found only in GSJ M35151-2 and M35151-3. Titanite is euhedral to subhedral < 0.2 mm in length. Spinel is green and subhedral in form (0.2-0.3 mm in grain size). Pentlandite occurs as lamellae in pyrrhotite.

## **Mineral chemistry**

Chemical analyses of the minerals were performed on a JEOL JXA-8800R electron microprobe analyzer at AIST. Accelerating voltage and specimen current were kept at





Fig. 2. Back-scattered electron image of zoned amphibole (GSJ

M35151-2). Msd: magnesiosadanagaite; Prg: pargasite; Ttn:

titanite; Phl: phlogopite.

Table 1. Chemical compositions of amphiboles.

	GSJ M35151-1			GSJ M35151-2			GSJ M35151-3				
-	core	rim	rim	rim	core	rim	rim	rim	core	rim	rim
	Prg	Msd	Msd	Msd#	Prg	Msd#	Msd	Msd	Prg	Msd	Msd
SiO2	41.1	35.6	36.4	37.1	42.9	37.7	37.9	37.3	42.2	37.4	37.2
TiO₂	1.76	4.02	2.71	2.70	1.19	2.64	2.81	2.88	1.66	2.87	2.88
$Al_2O_3$	17.2	22.2	22.0	20.9	15.3	19.8	19.7	20.0	15.9	20.9	20.2
Cr <sub>2</sub> O <sub>3</sub>	0.00	0.00	0.02	0.01	0.05	0.02	0.03	0.00	0.00	0.01	0.00
FeO*	5.27	7.10	8.03	6.76	5.40	6.45	6.85	6.60	4.60	5.98	5.58
MnO	0.19	0.24	0.21	0.18	0.09	0.14	0.12	0.15	0.02	0.18	0.14
MgO	16.2	12.5	12.0	13.4	17.0	14.2	14.3	14.0	17.1	14.3	14.4
CaO	12.5	12.2	12.2	12.5	12.7	12.7	12.5	12.5	13.0	12.5	12.6
Na₂O	3.24	3.48	3.32	3.33	2.89	2.61	2.62	2.67	2.89	2.81	2.81
K₂O	0.24	0.57	0.57	0.49	0.74	1.48	1.37	1.24	0.87	1.28	1.19
F	0.37	0.28	0.27	0.29	0.20	0.16	0.17	0.16	0.34	0.24	0.25
CI	0.04	0.02	0.02	0.02	0.13	0.14	0.14	0.15	0.17	0.17	0.12
-O=F+Cl	0.17	0.10	0.11	0.12	0.11	0.10	0.10	0.10	0.18	0.14	0.14
Total	97.9	98.1	97.6	97.6	98.5	97.9	98.4	97.6	98.6	98.5	97.2
H <sub>2</sub> O**	1.91	1.93	1.92	1.92	1.98	1.96	1.96	1.94	1.90	1.93	1.91
Fe <sub>2</sub> O <sub>3</sub> ***	0.12	0.54	0.09	0.60	0.30	0.95	0.82	0.73	0.21	0.77	0.78
FeO***	5.17	6.61	7.95	6.22	5.13	5.59	6.11	5.94	4.41	5.29	4.88
Total	99.9	100.1	99.6	99.5	100.5	100.0	100.5	99.6	100.5	100.5	99.2
				Struct	ural formu	lae based	d on 23 O	atoms			
Si	5.882	5.173	5.324	5.395	6.105	5.470	5.477	5.435	6.002	5.384	5.416
<sup>[4]</sup> AI	2.118	2.827	2.676	2.605	1.895	2.530	2.523	2.565	1.998	2.616	2.584
ΣΤ	8.000	8.000	8.000	8.000	8.000	8.000	8.000	8.000	8.000	8.000	8.000
<sup>[6]</sup> Al	0.783	0.975	1.116	0.977	0.671	0.856	0.832	0.869	0.667	0.930	0.882
Ti	0.189	0.439	0.298	0.295	0.127	0.288	0.305	0.316	0.178	0.311	0.315
Cr	0.000	0.000	0.002	0.001	0.006	0.002	0.003	0.000	0.000	0.001	0.000
Fe <sup>3+</sup>	0.013	0.060	0.010	0.066	0.032	0.104	0.090	0.080	0.022	0.083	0.085
Fe <sup>2+</sup>	0.619	0.803	0.972	0.756	0.611	0.680	0.739	0.724	0.525	0.637	0.595
Mn	0.023	0.030	0.026	0.022	0.011	0.017	0.015	0.019	0.002	0.022	0.017
Mg	3.456	2.708	2.616	2.905	3.606	3.071	3.081	3.041	3.625	3.069	3.126
ΣC	5.083	5.015	5.040	5.022	5.064	5.018	5.065	5.049	5.019	5.053	5.020
ΣC-5	0.083	0.015	0.040	0.022	0.064	0.018	0.065	0.049	0.019	0.053	0.020
Ca	1.917	1.899	1.912	1.948	1.936	1.974	1.935	1.951	1.981	1.928	1.966
<sup>(B]</sup> Na	0.000	0.086	0.048	0.030	0.000	0.008	0.000	0.000	0.000	0.019	0.014
ΣΒ	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000	2.000
<sup>IAI</sup> Na	0.899	0.894	0.894	0.909	0.797	0.726	0.734	0.754	0.797	0.765	0.779
К	0.044	0.106	0.106	0.091	0.134	0.274	0.253	0.230	0.158	0.235	0.221
ΣΑ	0.943	1.000	1.000	1.000	0.931	1.000	0.987	0.984	0.955	1.000	1.000
Total cation	15.943	16.000	16.000	16.000	15.931	16.000	15.987	15.984	15.955	16.000	16.000
F	0.167	0.129	0.125	0.133	0.090	0.073	0.078	0.074	0.153	0.109	0.115
CI	0.010	0.005	0.005	0.005	0.031	0.034	0.034	0.037	0.041	0.041	0.030
ОН	1.823	1.866	1.870	1.862	1.879	1.893	1.888	1.889	1.806	1.850	1.855
Notes: Prg=	pargasite	e, Msd=m	agnesios	adanagai	te.						
# Chemical	composit	tions of m	agnesios	adanagai	te for the )	C-ray stud	y. *Tot	al iron as	FeO.		
** H <sub>2</sub> O calcu	lation ba	ised on a	n assump	tion of OI	+F+Cl=2	0 apfu.					
355 E o <sup>or</sup> /E of		ion hooo	1 on tho n			- A (O - I		4007			

15 kV and 12 nA on a Faraday cup, respectively. Beam diameter was 10  $\mu$ m for F and Cl analyses and 2  $\mu$ m for other element analyses. Synthetic quartz (for Si), rutile (Ti), corundum (Al), Cr<sub>2</sub>O<sub>3</sub> (Cr), MnO (Mn), hematite (Fe), periclase (Mg), wollastonite (Ca) and F-phlogopite (F), as well as natural albite (Na), adularia (K) and Cl-rich hastingsite (Cl) were used as standards. The Bence & Albee (1968) method was employed for matrix corrections. Detection limits for F and Cl were about 0.08 and 0.01 wt.% (3 $\sigma$  level), respectively.

### Amphibole

Table 1 shows representative analyses of amphiboles. The chemical formulae were calculated on the basis of 23 oxygens. The  $Fe^{3+}/Fe^{2+}$  ratios were estimated using the minimum ferric method described by Schumacher (1997).

Amphibole crystal consists of an <sup>[4]</sup>Al-poorer core (< 2.19 apfu) and <sup>[4]</sup>Al-richer rim (< 2.84 apfu). The core has a fairly homogeneous composition within a thinsection scale, *i.e.*, pargasitic with  $X_{Fe^{2+}}$  [ = Fe<sup>2+</sup>/(Fe<sup>2+</sup> + Mg)] = 0.12-0.16 (Fig. 3). Its <sup>[4]</sup>Al and Ti contents are



Fig. 3. [4]Al vs.  $X_{Fe^{2+}}$  plots for amphiboles from the Kasuga-mura area.

Table 3. X-ray powder diffraction data for magnesiosadanægaite.

	GSJ M	35151-1		GSJ M	35151-2
h k l	I d (Å)obs.	d (Å)calc.	1 a	(Å)obs.	d (Å)calc.
020	50 8.98	8.96	50	8.97	9.00
1 1 0	100 8.38	8.40	70	8.47	8.43
-1 1 1	30 4.92	4.92	30	4.92	4.93
040	30 4.49	4.48	20	4.50	4.50
1 1 1	20 3.97	3.97	10	3.97	3.99
-131			20	3.91	3.90
1 3 1	60 3.37	3.37	60	3.38	3.38
240	50 3.26	3.26	50	3.27	3.27
3 1 0	80 3.11*	3.12	70	3.13*	3.13
-311	10 3.06	3.05	10	3.04	3.05
221	40 2.93	2.93	50	2.94	2.94
330	25 2.81	2.80	30	2.82	2.81
-331	45 2.75	2.75	40	2.76	2.75
151	80 2.70	2.69	100	2.70	2.70
061	75 2.58	2.58	70	2.59	2.59
-202	90 2.56	2.56	100	2.57	2.56
-261			20	2.42	2.42
350	20 2.38	2.37	30	2.39	2.38
-351	80 2.34 —	2.34	-90	2.35 —	2.35
-421		2.34			2.34
-312	40 2.30	2.30	40	2.30 —	2.30
-171		2.29			2.30
-242	25 2.24	2.22	20	2.23	2.23
261	55 2.16	2.15	60	2.16	2.16
202	35 2.04	2.04	40	2.04 -	2.04
-402		l 2.04			2.04
351	60 2.00	2.01	20	2.02	2.01
190			10	1.957	1.958
-352	10 1.951	1.947			
5 1 0			10	1.901	1.899
-191	35 1.854	1.855	20	1.863	1.863
-172	10 1.833	1.843			
0 10 0			10	1.801	1.800
-133	40 1.683	1.692	20	1.694	1.695
-282		L 1.685	10	1.680	1.691
4 6 1	50 1.645	1.642	30	1.650	1.648
1 11 0	50 1.609	1.606	30	1.614	1.613
600		1.586			1.591
-153	70 1.587	(1.583	30	1.591 -	1.586
402	40 1.549	1.548	30	1.552	1.553
-263	45 1.520	1.519	40	1.525	1.522
551		1.495	30	1.502	1.501
0 12 0	20 1.501	1.493 (			
-661	35 1.442	1.440	60	1.447	1.445
-553	20 1.371	1.371	20	1.373	1.373
1 11 2	40 1.333	1.333	30	1.337	1.339
-751	30 1.313	1.313	30	1.318	1.317
-2 12 2	20 1.291	1.290	20	1.301	1.295
-134		1.285			
-404	20 1.285	l 1.279			
-5 11 2	20 1.200	1.199	20	1.204	1.203
	a = 9.875	5(9) Å	i	a = 9.905	5(9) Å
	b =17.92(	1) Å	l	5 =18.00	(1) Å
	c = 5.314	(6) Å	c	c = 5.322	2(5) Å
β=105.55(7)° β=105.47(7)°					
* Estimated from data with the external Si-standard,					
beacause of overlap by the 111 diffraction of Si-standard.					

1.84-2.19 and 0.11-0.20 apfu, respectively. Chemical variation in the rim is relatively small in a single rock specimen. The rim of amphibole ranges in composition from pargasite to magnesiosadanagaite (Fig. 3), and its <sup>[4]</sup>Al and Ti contents are 2.45-2.84 and 0.22-0.44 apfu, respectively. The rim shows slightly higher  $X_{Fe^{2+}}$  values (0.16-0.27) than the core (0.12-0.16) (Fig. 3). Both the core and rim have relatively high <sup>[A]</sup>Na (0.67-0.96 apfu) and low K contents of < 0.29 apfu. The K+<sup>[A]</sup>Na contents of the core and rim are 0.90-1.00 and 0.93-1.00 apfu, respectively, and Ca contents are over 1.85 apfu. Chlorine content is less than 0.19 wt.% for both the core and rim. The core possess a slightly higher amount of F (0.20-0.42 wt.%) than the rim (0.13-0.31 wt.%).

### Other minerals

Chemical compositions of some minerals coexisting with the amphibole are shown in Table 2 (It can be obtained from the authors or through the E.J.M. Editorial Office - Paris). Phlogopite shows highly variable Na<sub>2</sub>O contents, and its Na content is 0.19-1.59 apfu (O = 22) for GSJ M35151-1 and less than 0.24 apfu for the two other samples (Banno *et al.*, in prep.). The  $X_{Fe^{2+}}$  values of phlogopite and chlorite are 0.09-0.14 and 0.11-0.29, respectively.

Spinel belongs to the spinel-hercynite series with  $X_{Fe^{2+}}$  about 0.35 and contains ZnO up to 4.69 wt.%. Ilmenite contains minor geikielite (7-11 %) and pyrophanite (4 %) components. The meionite component in scapolite ranges from 51 to 53 %. Up to 1.58 wt.%  $Al_2O_3$  is present in titanite.

# Physical and optical properties of magnesiosadanagaite

Physical and optical properties of magnesiosadanagaite were examined for sample GSJ M35151-2. Magnesiosadanagaite is brownish black in the hand specimen, and brown with reddish tint in powdered form. It is brittle with an uneven fracture, has perfect {110} cleavage. The Vickers microhardness is 665-792 kg/mm<sup>2</sup> (100 g load). It corresponds to 5.5-6 on Mohs' hardness scale. Magnesiosadanagaite is optically biaxial positive with  $\alpha$ 1.674(2),  $\beta$  (calc.) 1.683 for 2V of 85°,  $\gamma$  1.694(2),  $2V(\text{meas.}) > 80^\circ$  and  $< 90^\circ$ ;  $Z \wedge c 20^\circ$  and Y = b. It is pleochroic with X = pale yellow, Y = yellowish brown and Z = reddish brown.

# X-ray crystallography of magnesiosadanagaite

Single crystal fragments of magnesiosadanagaite carefully handpicked from thin sections of GSJ M35151-1 and M35151-2 were used for X-ray study. Chemical compositions of the magnesiosadanagaite are presented in Table 1.

### X-ray powder study

The X-ray powder diffraction data obtained with a 114.6 mm Gandolfi camera (at the National Science Museum) using Cu/Ni radiation are given in Table 3. Observed *d*-values were corrected by the method proposed by Toraya (1993). Peaks were indexed by reference to the data of hornblende (Borg & Smith, 1969) and potassic-magnesiosadanagaite (Shimazaki *et al.*, 1984). The unit cell parameters obtained from the present data are *a* = 9.875(9), *b* = 17.92(1), *c* = 5.314(6) Å,  $\beta$  = 105.55(7)° and V = 906(1) Å<sup>3</sup> for GSJ M35151-1 and *a* = 9.905(9), *b* = 18.00(1), *c* = 5.322(5) Å,  $\beta$  = 105.47(7)° and V = 915(1) Å<sup>3</sup> for GSJ M35151-2. Due to the lower Fe<sup>2+</sup> and K contents, cell volumes for both samples are distinctly smaller than that (926 Å<sup>3</sup>) measured for potassic-magnesiosadanagaite (K = 0.75 apfu: X<sub>Fe<sup>2+</sup></sub> = 0.43, Shimazaki *et al.*, 1984).

Table 4. Crystallographic data and experimental details of single crystal studies on magnesiosadanagaite.

	GSJ M35151-1	GSJ M35151-2
a (Å)	9.869(3)	9.906(2)
b (Å)	17.933(7)	17.971(5)
c (Å)	5.322(2)	5.3190(10)
β (°)	105.29(3)	105.48(2)
V (Å <sup>3</sup> )	908.6(6)	912.5(4)
Space group	C2/m	C2/m
Z	2	2
D <sub>calc</sub> (g/cm <sup>3</sup> )	3.179	3.171
μ (cm <sup>-1</sup> )	2.191	2.194
Crystal dimension (mm)	0.12 x 0.12 x 0.05	0.17 x 0.17 x 0.07
Diffractometer	Rigaku AFC-7R	Rigaku AFC-7R
Radiation	MoK $\alpha$ (graphite)	MoK α (graphite)
Scan mode, rate (°/ min in ω)	2 <del>0</del> -ω, 16	2θ-ω, 8
2θ range	7.9 - 60.0	7.9 — 55.0
Reflection range	-13 ≤ h ≤ 13,	-12≤h≤7,
	0 ≤ k ≤ 25,	0 ≤ k ≤ 23,
	-7≤l≤3,	-6 ≤ I ≤ 6,
No. of measured reflections	1653	1307
No. unique reflections	1374	1082
No. of observed reflections [F $^{2} > 2\sigma(F^{2})$ ]	1009	962
R int	3.3 %	1.7 %
Variable parameters	103	102
$R = 1 [F^2 > 2\sigma(F^2)], R = 1 (all reflections)$	4.2 %, 7.1 %	2.8 %, 3.3 %
wR 2 (all reflections)	14.0 %	12.8 %
Weghting parameters, a, b	0.1, 0	0.1, 0
Goodness of Fit	0.947	1.109
Final Δρ <sub>max</sub> (e/ Å ³)	0.780	0.472
Final Δρ <sub>min</sub> (e/Å <sup>3</sup> )	-0.895	-0.828
$R = \Sigma   F_o  -  F_c   / \Sigma  F_o $		
wR 2 = { $\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]$ } <sup>0.5</sup>		
$w = 1 / [\sigma^2(F_o^2) + (aP)^2 + bP]$		
$P = [2F_c^2 + F_o^2] / 3$		

### **Structure refinement**

Single-crystal diffraction data were collected and refined for two samples, GSJ M35151-1 and M35151-2. Experimental details pertaining to the collection are given in Table 4. The data reductions to Fo<sup>2</sup> with corrections for Lorentz, polarization and absorption ( $\psi$ -scan procedure) were made with a computer program written by Dr. Kazumasa Sugiyama of the University of Tokyo. The crystal structures were refined with SHELXL-97 (Sheldrick, 1997) based on Fo<sup>2</sup> against all reflections with the weighting function shown in Table 4. Scattering factors for neutral atoms were taken from the International Tables for X-ray Crystallography Volume C (1992). The numbers of equivalent reflections collected from the samples GSJ M35151-1 and M35151-2 are 279 and 225, respectively. The refinements for GSJ M35151-1 and M35151-2 converged with R1  $[F^2 > 2\sigma(F^2)] = 0.0422$  and 0.0277, respectively and R1 (all reflections) = 0.0710 and 0.0329, respectively. The results of the refinements were summarized in Table 4. The final atomic coordinates, cation occupancies, equivalent isotropic and anisotropic displacement parameters are given in Table 5. Selected interatomic distances and angles are in Table 6 (It can be obtained from the authors or through the E.J.M. Editorial Office - Paris).

The occupancy factors of Al in the T(2) site, <sup>T(2)</sup>Al(apfu), were calculated for both samples using equation (5) in Oberti *et al.* (1995), which was corrected as follows; <sup>T(2)</sup>Al = [<T(2)-O>-<T(2)-O><sub>c</sub>] x 35.2592 (Sokolova *et al.*, 2000; Oberti, pers. comm.). The results, <sup>T(2)</sup>Al (apfu) = 0.47 and 0.35, are both smaller than the values calculated from the differences between tetrahedral Al and Al in the T(1) site, <sup>[4]</sup>Al (apfu)-<sup>T(1)</sup>Al (apfu) = 0.58 and 0.62 for GSJ M35151-1 and M35151-2, respectively. Equation (1) reported in Oberti *et al.* (1995) to calculate  $\langle T(2)-O \rangle_c$  was obtained from a regression of lower-Al amphiboles and may not be applicable for these higher Al-amphiboles.

Titanium is usually considered as an octahedral cation in most amphiboles, and most structural studies of amphiboles with low Ti contents (< 0.20 apfu) have assigned Ti to the M(2) site. Recently, Oberti et al. (1992) and Hawthorne et al. (1998) studied the behavior of Ti in sodiccalcic and sodic amphiboles. They showed that in these minerals the entry of Ti occurs primarily in the substitution,  $M^{(1)}Ti^{4+} + 2O^{(3)}O^{2-} \rightarrow M^{(1)}(Mg, Fe)^{2+} + 2O^{(3)}OH^{-}$ , and that the M(1)-O(3) distance decreases markedly with increasing Ti content in the structure. Sokolova et al. (2000) pointed out that dehydroxylated amphiboles with OH + F < 2 apfu and significant Ti<sup>4+</sup> and Fe<sup>3+</sup> at M(1) [and M(3)] show  $M(1)-O(3) \ll M(1)-O$ . The magnesiosadanagaite in this study shows that M(1)-O(3) is not less than  $\langle M(1)-O \rangle$ (Table 6), indicating that the magnesiosadanagaite is not dehydroxylated and has no  $Ti^{4+}$  at the M(1) site.

The O(5)-O(6)-O(5) angles for GSJ M35151-1 and M35151-2 are 160.4° and 161.8°, respectively. The studied samples have the lowest values of the O(5)-O(6)-O(5) angle ever reported in C2/m amphibole (*cf.* Fig. 3 in Sokolova *et al.*, 2000), indicating maximal kinking of the double-chain of tetrahedra.

### Discussion

Potassicsadanagaite and potassic-magnesiosadanagaite, described initially as "sadanagaite" and "magnesiosadana-

Table 5. Final atomic coordinates, cation occupancies and displacement parameters (Å<sup>2</sup>) for magnesiosadanagaite.

GSJ 10351	151-1					
Site	Occupancy (apf	ົນ)	x	у.	z	Ueq
T(1)	1.97Si+2.03Al		0.27999(10)	0.08616(5)	0.30473(19)	0.0077(2)
T(2)	3.43Si+0.57Al		0.29136(10)	0.17386(5)	0.81769(18)	0.0080(2)
Man	1.62Ma+0.38Fe		0.0000	0.08999(7)	0.5000	0.0079(3)
Mizi	0.53Ma+0.19Fe	+0.98AI+0.30Ti	0.0000	0.17726(7)	0.0000	0.0104(3)
M(3)	0.75Ma+0.25Fe	•	0.0000	0.0000	0.0000	0.0080(3)
M(4)	1.95Ca+0.02Mr	+0.03Na	0.0000	0.28122(5)	0.5000	0.0109(2)
A (2)	0.91Na+0.09K		0.0000	0.4776(4)	0.0000	0.068(3)
	40		0.1050(3)	0.09056(15)	0.2122(5)	0.0132(5)
	40		0 1182(3)	0 17486(13)	0 7402(5)	0.0108(5)
	1 870±0 13E		0.1083(4)	0.0000	0 7139(7)	0.0112(7)
	40		0.7700(4)	0.0000	0.7103(7)	0.012(7)
	40		0.3700(3)	0.20190(14)	0.1921(5)	0.0120(5)
	40		0.3522(3)	0.14100(14)	0.1176(5)	0.0130(5)
	40		0.3425(3)	0.11659(15)	0.6141(5)	0.0143(5)
0(/)	20		0.3368(4)	0.0000	0.2715(7)	0.0154(7)
н	1.87H		0.173(15)	0.0000	0.85(3)	0.15(7) *
	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>23</sub>	U <sub>13</sub>	U <sub>12</sub>
T(1)	0.0092(5)	0.0056(4)	0.0089(5)	0.0002(3)	0.0036(4)	-0.0008(3)
T(2)	0.0098(4)	0.0060(4)	0.0096(4)	0.0002(3)	0.0050(3)	0.0003(3)
M(1)	0.0111(6)	0.0064(6)	0.0078(6)	0.000	0.0053(5)	0,000
M(2)	0.0121(6)	0.0090(6)	0.0109(6)	0.000	0.0047(5)	0.000
M(3)	0.0106(8)	0.0061(7)	0.0081(8)	0.000	0.0039(6)	0.000
M(4)	0.0152(5)	0.0076(4)	0.0124(5)	0.000	0.0078(4)	0.000
A	0.058(4)	0.080(7)	0.087(5)	0.000	0.057(4)	0.000
0(1)	0.0123(11)	0.0173(12)	0.0113(12)	-0.0011(9)	0.0054(10)	-0.0040(9)
02	0.0115(11)	0.0087(11)	0.0128(11)	0.0010(8)	0.0039(9)	0.0010(9)
0(3)	0.0104(15)	0.0088(15)	0.0149(17)	0.000	0.0042(14)	0.000
0(4)	0.0171(11)	0.0083(11)	0.0147(12)	0.0007(9)	0.0081(10)	-0.0011(9)
0(5)	0.0136(12)	0.0110(11)	0.0154(12)	0.0021(9)	0.0056(10)	-0.0008(9)
0(6)	0.0125(12)	0.0136(12)	0.0172(13)	-0.0039(10)	0.0044(10)	0.0009(9)
	0.0164(18)	0.0100(12)	0.0188(18)	0.000	0.0068(15)	0.0000(0)
GQ   M251	151.0	0.0122(10)	0.0100(10)	0.000	0.0000(10)	0.000
033 1033 1	101-2					
	/ 1 /				_	
Site	Occupancy (apt	u)	X	<u>y</u>	Z	Ded O
T(1)	2.10Si+1.90Al	u)	x 0.27942(7)	y 0.08595(4)	z 0.30443(14)	0.0066(3)
T(1) T(2)	Occupancy (apt 2.10Si+1.90Al 3.37Si+0.63Al	u)	x 0.27942(7) 0.29054(7)	y 0.08595(4) 0.17353(4)	z 0.30443(14) 0.81600(13)	0.0066(3) 0.0068(3)
Site T(1) T(2) M(1)	Occupancy (apt 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe	u)	x 0.27942(7) 0.29054(7) 0.0000	y 0.08595(4) 0.17353(4) 0.08973(5)	z 0.30443(14) 0.81600(13) 0.5000	0.0066(3) 0.0068(3) 0.0074(3)
T(1) T(2) M(1) M(2)	Occupancy (apt 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe	u) 9 9+0.86Al+0.29Ti	x 0.27942(7) 0.29054(7) 0.0000 0.0000	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5)	z 0.30443(14) 0.81600(13) 0.5000 0.0000	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3)
T(1) T(2) M(1) M(2) M(3)	2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe	u) 9+0.86Al+0.29Ti 9	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.0000	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3)
T(1) T(2) M(1) M(2) M(3) M(4)	2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na	u) 9+0.86Al+0.29Ti 9 1+0.02Mn	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.0000 0.5000	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0096(3)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m)	2:10Si+1:90Al 3:37Si+0:63Al 1:66Mg+0:34Fe 0:60Mg+0:25Fe 0:81Mg+0:19Fe 1:97Ca+0:01Na 0:73Na+0:27K	9 9+0.86Al+0.29Ti 9 1+0.02Mn	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.0000	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.0000 0.5000 0.0000	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0096(3) 0.111(2)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1)	2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 4O	u) 9 9+0.86Al+0.29Ti 9 9 9+0.02Mn	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.10562(19)	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.5000 0.0000 0.2147(4)	0.0066(3) 0.0068(3) 0.0074(3) 0.00113(3) 0.0056(3) 0.0096(3) 0.111(2) 0.0119(4)
Site       T(1)       T(2)       M(1)       M(2)       M(3)       M(4)       A (2/m)       O(1)       O(2)	Cccupancy (ap) 2.105i+1.90Al 3.375i+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40	9 9+0.86Al+0.29Ti 9 9+0.02Mn	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19)	y 0.08595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.5000 0.2147(4) 0.7371(4)	0.0066(3) 0.0068(3) 0.0074(3) 0.0074(3) 0.0056(3) 0.0096(3) 0.111(2) 0.0119(4) 0.0101(4)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3)	Cocupancy (ap) 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 1.90C+0.07F+0	9 9+0.86Al+0.29Ti 9 1+0.02Mn 0.03Cl	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3)	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.5000 0.2147(4) 0.7371(4) 0.7157(5)	0.0066(3) 0.0068(3) 0.0074(3) 0.0074(3) 0.00756(3) 0.0096(3) 0.111(2) 0.0119(4) 0.0101(4) 0.0140(6)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(2) O(3) O(4)	Cocupancy (ap) 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 1.900+0.07F+0 40	9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.38863(19)	y 0.06595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4)	0.0066(3) 0.0068(3) 0.0074(3) 0.0074(3) 0.0056(3) 0.0096(3) 0.111(2) 0.0119(4) 0.0110(4) 0.0112(4)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5)	Cocupancy (ap) 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 1.90O+0.07F+0 40 40	uy +-0.86Al+0.29Ti +-0.02Mn 	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36869(19) 0.35101(18)	y 0.08595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10) 0.25114(10) 0.14053(11)	z 0.30,443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(4) 0.0119(4) 0.0119(4) 0.01114(2) 0.0112(4) 0.0112(4)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6)	Occupancy (ap) 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 1.90O+0.07F+0 40 40 40	9 9+0.86Al+0.29Ti 9 9 9 9 9 9 0.03Cl	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36869(19) 0.35101(18) 0.34361(18)	y 0.08595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.25114(10) 0.25114(10) 0.14053(11) 0.11710(11)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.5000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0056(3) 0.0096(3) 0.111(2) 0.0119(4) 0.0119(4) 0.0112(4) 0.0122(4) 0.0131(4)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7)	Occupancy (ap) 2.105i+1.90Al 3.375i+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 40 40 40 40 40 40 40 20	uy +0.86Al+0.29Ti +40.02Mn +40.02Mn	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.3858(19) 0.35101(18) 0.335101(18) 0.3372(3)	y 0.06595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.11710(11) 0.0000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.625(5)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0113(3) 0.0113(3) 0.0113(4) 0.0119(4) 0.01119(4) 0.0112(4) 0.01122(4) 0.0131(4) 0.0131(59(6)
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H	Cocupancy (ap) 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 40 40 40 40 20 1.90H	uy ++0.86Al+0.29Ti ++0.02Mn ++0.02Mn	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36869(19) 0.36101(18) 0.34361(18) 0.34361(18) 0.3372(3) 0.189(5)	y 0.06595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.11710(11) 0.0000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.2047(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2766(5) 0.750(8)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0056(3) 0.111(2) 0.0119(4) 0.0101(4) 0.0112(4) 0.0122(4) 0.0131(4) 0.0159(6) 0.000(10)*
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H	Cocupancy (ap) 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 1.90C+0.07F+0 40 40 40 20 1.90H U.	uy 9 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1 9 1	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36868(19) 0.36	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.17438(10) 0.25114(10) 0.25114(10) 0.14053(11) 0.11710(11) 0.0000 0.0000 U <sub>20</sub>	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2766(5) 0.750(8) U_a	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0096(3) 0.111(2) 0.0119(4) 0.0101(4) 0.0101(4) 0.0122(4) 0.0159(6) 0.000(10) <sup>4</sup>
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(1)	Occupancy (ap) 2.105i-1.90Al 3.375i+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.3Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 40 40 40 40 40 40 40 40	U) ++0.86Al+0.29Ti ++0.02Mn 0.03Cl U <sub>22</sub> 0.0069(4)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.1088(3) 0.36569(19) 0.36569(19) 0.35101(18) 0.36569(19) 0.35101(18) 0.3372(3) 0.189(5) U <sub>33</sub> 0.069(4)	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.14053(11) 0.14053(11) 0.10000 0.0000 U <sub>23</sub> 0.0000(2)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2756(5) 0.750(8) U 13 0.00222(3)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0114(4) 0.0119(4) 0.0119(4) 0.0112(4) 0.0112(4) 0.0131(4) 0.0132(4) 0.0159(6) 0.000(10)*
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) T(2)	Occupancy (ap) 2.10Si+1.90Al 3.37Si+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 40 40 40 40 20 1.90CH U <sub>11</sub> 0.0062(4) 0.0072(4)	uy + 0.86Al+0.29Ti + 0.02Mn 0.03Cl U <sub>22</sub> 0.0069(4) 0.0069(4)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.3669(19) 0.356101(18) 0.3372(3) 0.3372(3) 0.189(5) U <sub>33</sub>	y 0.06595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.28043(11) 0.17438(10) 0.0000 0.25114(10) 0.10000 0.25114(10) 0.10000 0.25114(10) 0.10000 U <sub>25</sub> 0.0000(2) 0.0000(2)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2766(5) 0.2766(5) U <sub>19</sub> 0.00022(3) 0.00022(3)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.111(2) 0.0119(4) 0.0101(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.0131(4) 0.0122(4) 0.0031(4) 0.0005(2) U <sub>12</sub>
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) T(1) T(2) M(1) M(2) M(3) M(4) D(2) D(2) D(2) D(2) M(3) M(4) D(2) D(2) D(2) M(3) M(4) D(2) M(3) M(4) D(2) D(2) M(3) M(4) D(2)	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Nz       0.73Na+0.27K       40       40       40       40       40       40       40       40       40       40       40       40       40       40       20       1.900H       U11       0.0062(4)       0.0072(4)	U) + + +0.86AI+0.29Ti + +0.02Mn 0.03Cl U_2 0.0069(4) 0.0069(4) 0.0069(4) 0.0069(4)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36869(19) 0.35101(18) 0.36869(19) 0.35101(18) 0.3372(3) 0.189(5) U_{33} 0.0069(4) 0.0070(4) 0.0070(4)	y 0.08595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.14053(11) 0.11710(11) 0.0000 0.0000 0.0000 U <sub>23</sub> 0.0000(2) 0.0003(2)	z 0.30,443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7157(5) 0.7914(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.2766(5) 0.2766(5) 0.2765(6) U <sub>13</sub> 0.0022(3) 0.0032(3) 0.0032(3) 0.0032(4)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0056(3) 0.0096(3) 0.111(2) 0.0119(4) 0.0110(4) 0.0112(4) 0.0122(4) 0.0131(4) 0.0159(6) 0.0000(12) U <sub>12</sub> -0.0008(2) 0.0000(2)
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(2) M(2) M(3) M(3) M(4) O(1) O(2) M(3) M(4) O(1) O(2) M(3) M(4) O(1) O(2) M(3) M(4) O(1) O(2) M(3) M(4) O(1) O(2) M(3) M(4) O(1) O(2) M(4) O(1) O(2) M(4) O(2) M(4) O(1) O(2) O(3) O(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(1) O(2) O(3) O(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) O(3) O(4) O(7) D(7) M(4) O(7) M(4) O(7) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(2) M(4) O(7) M(4) O(7) M(4) O(7) M(4) O(7) M(4) O(7) M(4) O(7) M(4) O(7) M(4) M(4) M(4) M(4) M(4) M(4) M(4) M(4) M(4) M(4) M(4) M(7)	Occupancy (ap) 2.105i+1.90Al 3.375i+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.3Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 40 40 40 40 40 40 40 40	U) +++0.86Al+0.29Ti +++0.02Mn 0.03Cl U_2 0.0069(4) 0.0069(4) 0.0069(5) 0.0065(5) 0.0065(5)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.3658(19) 0.36101(18) 0.3658(19) 0.36101(18) 0.3625(19) 0.372(3) 0.189(5) U <sub>31</sub> 0.0069(4) 0.0070(4) 0.0069(4) 0.0062(6) 0.0116	y 0.06595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.08934(11) 0.17438(10) 0.25114(10) 0.14053(11) 0.14053(11) 0.111710(11) 0.0000 U <sub>23</sub> 0.0000(2) 0.0003(2) 0.0003(2) 0.000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2750(8) U <sub>13</sub> 0.0022(3) 0.0032(3) 0.0040(4) 0.0040(4)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0056(3) 0.0111(2) 0.0119(4) 0.0119(4) 0.0112(4) 0.01122(4) 0.01122(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.0158(6) 0.0001(2) 0.00008(2) 0.00006(2) 0.0000(2) 0.0000(2)
Site T(1) T(2) M(2) M(3) M(4) M(3) M(4) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(1) M(2) M(2) M(2) M(2) M(3) M(3) M(3) M(3) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Na       0.73Na+0.27K       40       40       40       40       40       40       40       40       40       40       40       40       40       20       1.90H       U11       0.0082(4)       0.0072(4)       0.0085(5)       0.0119(5)	U) ++0.86Al+0.29Ti ++0.02Mn 0.03Cl U <sub>22</sub> 0.0069(4) 0.0069(4) 0.0065(5) 0.0113(5) 0.0013(5)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36863(19) 0.36863(19) 0.35101(18) 0.3372(3) 0.36863(19) 0.3372(3) 0.369(5) U <sub>33</sub> 0.0069(4) 0.0070(4)0	y 0.06595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.2804(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.11710(11) 0.0000 U <sub>23</sub> 0.0000(2) 0.0003(2) 0.000 0.000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.7157(5) 0.757(5) 0.757(5) 0.757(5) 0.757(6) U <sub>15</sub> 0.0022(3) 0.0040(4) 0.0047(4) 0.0047(4) 0.0047(4) 0.0047(4)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0056(3) 0.0119(4) 0.0119(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.0121(4) 0.0122(4) 0.0121(4) 0.0122(4) 0.0001(0)* U <sub>12</sub> -0.0008(2) 0.0000(2) 0.0000
Site T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) O(7) H T(1) T(2) M(1) M(2) M(1) M(2) M(1) M(2) M(2) M(2) M(2) M(2) M(3) O(2) O(3) O(4) O(5) O(6) O(7) M(1) M(2) M(2) M(2) M(3) M(4) M(3) M(4) M(3) M(4) M(3) M(4) M(2) M(3) M(4) M(3) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(2) M(4) M(4) M(2) M(4) M(2) M(4) M(4) M(2) M(4)	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Na       0.73Na+0.27K       40       20       20       20       0.0072(4)       0.0075(5)       0.0075(7)       0.0075(7)	U) +++0.86Al+0.29Ti ++0.02Mn 0.03Cl U₂ 0.0069(4) 0.0069(4) 0.0065(5) 0.0113(5) 0.0050(6) 0.0050(6)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36869(19) 0.35101(18) 0.36869(19) 0.35101(18) 0.34361(18) 0.34361(18) 0.34361(18) 0.34361(18) 0.34361(18) 0.34361(18) 0.3689(5) U <sub>33</sub>	y 0.08595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.11710(11) 0.0000 U <sub>20</sub> 0.0000 U <sub>20</sub> 0.0000(2) 0.0003(2) 0.000 0.000 0.000	z 0.30,443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.5000 0.2147(4) 0.7371(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.6125(3) 0.2766(5) 0.750(8) U <sub>13</sub> 0.0032(3) 0.0032(3) 0.0040(4) 0.0047(4) 0.0047(4) 0.0047(4) 0.0047(4) 0.0047(4) 0.0047(4) 0.0011(5)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0056(3) 0.0096(3) 0.111(2) 0.0119(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.0131(4) 0.0122(4) 0.00122(4) 0.0000(10)* U12 -0.0008(2) 0.0000 0.0000
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(3) M(4) M(4)	Occupancy (ap) 2.105i+1.90Al 3.375i+0.63Al 1.66Mg+0.34Fe 0.60Mg+0.25Fe 0.81Mg+0.19Fe 1.97Ca+0.01Na 0.73Na+0.27K 40 40 40 40 40 40 40 40 40 40	U) +++0.86Al+0.29Ti +++0.02Mn 0.03Cl U₂ 0.0069(4) 0.0069(4) 0.0069(4) 0.0069(5) 0.0113(5) 0.0113(5) 0.0059(6) 0.0059(4)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.36105(3) 0.36101(18) 0.36263(19) 0.35101(18) 0.36263(19) 0.35101(18) 0.36263(19) 0.35101(18) 0.3672(3) 0.189(5) U_{31} 0.0069(4) 0.0070(4) 0.00069(4) 0.00109(4) 0.00109(4) 0.00109(4)	y 0.08595(4) 0.17353(4) 0.28973(5) 0.17709(5) 0.2000 0.28089(4) 0.5000 0.28934(11) 0.17438(10) 0.25114(10) 0.25114(10) 0.14053(11) 0.14053(11) 0.11710(11) 0.0000 0.0000 U <sub>23</sub> 0.0000(2) 0.0000 0.0000 0.000 0.0000 0.0000 0.0000 0.000 0.000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2750(8) U <sub>13</sub> 0.0022(3) 0.0040(4) 0.0047(4) 0.0062(3) 0.0062(3) 0.0062(3)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.1113(3) 0.0119(4) 0.0119(4) 0.0119(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.0158(6) 0.0001(2) 0.0000(2) 0.0000(2) 0.0000 0.0000 0.0000
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(3) M(4) A (2/m) M(3) M(4) A (2/m) M(3) M(4) A (2/m) M(3) M(4) A (2/m) M(4) M(3) M(4) A (2/m) M(4) M(3) M(4) M(4) M(3) M(4	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Na       0.73Na+0.27K       40       40       40       40       40       40       20       1.90H       U <sub>11</sub> 0.0082(4)       0.0072(4)       0.0075(7)       0.0119(5)       0.0075(7)	U) ++0.86AI+0.29Ti ++0.02Mn 0.03Cl U₂ 0.0069(4) 0.0069(4) 0.0069(5) 0.0113(5) 0.0050(6) 0.0059(4) 0.0050(6) 0.0059(4) 0.205(6)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.000582(19) 0.11888(19) 0.1088(3) 0.36563(19) 0.35101(18) 0.36563(19) 0.35101(18) 0.3372(3) 0.3695(11) U_{33} 0.00059(4) 0.0070(4) 0.0042(6) 0.0117(6) 0.0042(6) 0.019(4) 0.089(3)	y 0.06595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.28089(4) 0.5000 0.28934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.11710(11) 0.0000 U <sub>25</sub> 0.0000(2) 0.0003(2) 0.000 0.000 0.000 0.000 0.000 0.000 0.000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.6125(3) 0.2766(5) 0.750(6) U <sub>15</sub> 0.00022(3) 0.0040(4) 0.0047(4) 0.0047(4) 0.0062(2) 0.062(2)	0.0066(3) 0.0068(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0056(3) 0.0119(4) 0.0119(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.01212(4) 0.01212(4) 0.01212(4) 0.0121(4) 0.0122(4) 0.000(10)* U <sub>12</sub> -0.0008(2) 0.0000 0.000 0.000 0.000
Site       T(1)       T(2)       M(3)       M(3)       M(4)       A (2/m)       O(1)       O(3)       O(4)       O(5)       O(6)       O(7)       H       T(1)       T(2)       M(1)       M(2)       M(3)       M(4)       A       O(1)	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.60Mg+0.25Fe       0.73Na+0.27K       40       40       40       40       40       40       40       40       40       40       40       40       40       20       1.900H       0.0082(4)       0.0072(4)       0.0075(7)       0.019(5)       0.0075(7)       0.0093(10)	U) +++0.86Al+0.29Ti +++0.02Mn 0.03Cl U₂ 0.0069(4) 0.0069(4) 0.0069(4) 0.0050(6) 0.0050(6) 0.0050(6) 0.0050(6) 0.0050(6) 0.0050(6) 0.0165(10)	$\begin{array}{c} x \\ 0.27942(7) \\ 0.29054(7) \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.0000 \\ 0.10562(19) \\ 0.10562(19) \\ 0.10562(19) \\ 0.1086(3) \\ 0.36863(19) \\ 0.36863(19) \\ 0.35101(18) \\ 0.3372(3) \\ 0.35101(18) \\ 0.3372(3) \\ 0.189(5) \\ U_{30} \\ 0.0059(4) \\ 0.00052(6) \\ 0.00109(4) \\ 0.0052(6) \\ 0.0109(4) \\ 0.0059(3) \\ 0.0099(9) \end{array}$	y 0.08595(4) 0.17353(4) 0.08973(5) 0.17709(5) 0.0000 0.28089(4) 0.5000 0.08934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.14053(11) 0.14053(11) 0.14053(11) 0.14053(11) 0.14053(11) 0.0000 0.0000 U <sub>25</sub> 0.00000 0.0000 0.0000 0.000000 0.0000000 0.00000 0.00000 0.00000 0.00000 0	$\begin{array}{c} z \\ 0.30443(14) \\ 0.81600(13) \\ 0.5000 \\ 0.0000 \\ 0.5000 \\ 0.5000 \\ 0.0000 \\ 0.2147(4) \\ 0.7157(5) \\ 0.714(4) \\ 0.7157(5) \\ 0.7914(4) \\ 0.1155(3) \\ 0.6125(3) \\ 0.750(6) \\ U_{19} \\ \hline 0.0022(3) \\ 0.0032(3) \\ 0.0040(4) \\ 0.0047(4) \\ 0.0062(2) \\ 0.0062(2) \\ 0.0032(7) \\ \end{array}$	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.01114(2) 0.0119(4) 0.0119(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.0121(4) 0.0123(4) 0.0123(4) 0.0123(4) 0.0159(6) 0.00005(2) 0.0000(2) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(3) M(4) A O(1) O(2) O(1) O(2) O(2) O(1) O(2) O(2) O(1) O(2) O(2) O(1) O(2	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Na       0.73Na+0.27K       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       90       1.90H       U1       0.0062(4)       0.0075(7)       0.0119(5)       0.019(4)       0.603(2)       0.0075(10)       0.0076(9)	U) +++0.86Al+0.29Ti +++0.02Mn 0.03Cl U2 0.0069(4) 0.0069(4) 0.0065(5) 0.0113(5) 0.0113(5) 0.0059(6) 0.0059(6) 0.0059(4) 0.205(6) 0.0165(10) 0.0124(9)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.35101(18) 0.3658(19) 0.35101(18) 0.3686(19) 0.35101(18) 0.335101(18) 0.3372(3) 0.189(5) U_{33} 0.0069(4) 0.0070(4) 0.0062(6) 0.0117(6) 0.0109(4) 0.0099(9) 0.0099(9)	y       0.06595(4)       0.17353(4)       0.08973(5)       0.17709(5)       0.0000       0.28089(4)       0.5000       0.2804(11)       0.17438(10)       0.0000       0.25114(10)       0.17170(11)       0.0000       U <sub>23</sub> 0.0000(2)       0.0000(2)       0.0000       0.0000(2)       0.0000(2)       0.0000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2765(5) 0.750(8) U <sub>13</sub> 0.0022(3) 0.0032(3) 0.0047(4) 0.0011(5) 0.0062(2) 0.0030(7) 0.0030(7) 0.0013(7)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0113(3) 0.0113(3) 0.0113(3) 0.0113(4) 0.0119(4) 0.01119(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.0000(2) 0.0000(2) 0.0000(2) 0.0000(2) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(3) M(4) A O(1) O(2) O(3)	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Na       0.73Na+0.27K       40       40       40       40       40       40       40       40       0.0052(4)       0.0072(4)       0.0075(7)       0.019(4)       0.0053(2)       0.0055(10)       0.0076(9)       0.0162(15)	U) ++0.86Al+0.29Ti ++0.02Mn 0.03Cl U <sub>22</sub> 0.0069(4) 0.0069(4) 0.0069(5) 0.0113(5) 0.0050(6) 0.0055(6) 0.0165(10) 0.0162(19) 0.0162(19) 0.0119(13)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36863(19) 0.35101(18) 0.36863(19) 0.35101(18) 0.3372(3) 0.36863(19) 0.35101(18) 0.3372(3) 0.3695(5) U_{33} 0.0069(4) 0.0070(4) 0.0062(6) 0.0117(6) 0.0042(6) 0.0117(6) 0.0059(3) 0.0099(9) 0.0099(9) 0.0099(9) 0.0141(13)	y 0.06595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.28089(4) 0.5000 0.28934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.11710(11) 0.0000 U <sub>23</sub> 0.0000(2) 0.0003(2) 0.0000 0.000 0.000 0.000 0.000 0.000 0.0000 0.000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2766(5) 0.750(8) U <sub>15</sub> 0.00022(3) 0.0040(4) 0.0047(4) 0.0047(4) 0.0030(7) 0.0030(7) 0.0031(7) 0.0044(10)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0113(3) 0.0056(3) 0.111(2) 0.0119(4) 0.0119(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.0001(0)* U <sub>12</sub> -0.0008(2) 0.0000(10)* U <sub>12</sub> -0.0008(2) 0.0000 0.000 0.000 0.000 0.000 0.000 0.00000 0.000000
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(4) A A O(1) O(2) O(3) O(1) O(2) O(1) O(2) O(3) O(1) O(2) M(4) A A O(1) O(2) M(3) M(4) A O(2) M(3) M(4) A O(1) O(2) O(3) O(1) O(2) O(3) O(4) O(3) O(4) O(3) O(4) O(3) O(4) O(2) M(4) M(3) M(4) A O(2) M(4) O(3) O(6) O(7) D(7) M(2) M(3) M(4) O(7) D(6) O(7) D(7	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.60Mg+0.25Fe       0.73Na+0.27K       40       40       40       40       40       40       40       40       40       40       40       40       40       20       1.900H       0.0072(4)       0.0072(4)       0.0075(7)       0.019(5)       0.0075(7)       0.0055(10)       0.0075(7)       0.0192(5)       0.0075(7)       0.0075(7)       0.0192(5)       0.0075(7)       0.0075(7)       0.0075(7)       0.0075(7)       0.0076(9)       0.0162(15)       0.0152(5)	U) H-0.86Al+0.29Ti H+0.02Mn 0.03Cl U <sub>22</sub> 0.0069(4) 0.0069(4) 0.0085(5) 0.0113(5) 0.0050(6) 0.0050(6) 0.0025(6) 0.0050(6) 0.0025(7) 0.0124(9) 0.0119(13) 0.0024(9)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.10562(19) 0.1088(3) 0.36863(19) 0.36863(19) 0.36863(19) 0.35101(18) 0.335101(18) 0.335101(18) 0.335101(18) 0.3372(3) 0.189(5) U_{33} 0.0069(4) 0.0070(4) 0.0069(4) 0.0019(4) 0.0099(9) 0.0042(6) 0.0099(9) 0.0041(13) 0.0029(9) 0.0141(13) 0.0125(9)	y       0.08595(4)       0.17353(4)       0.08973(5)       0.17709(5)       0.0000       0.28089(4)       0.5000       0.28089(4)       0.5000       0.28089(4)       0.5000       0.28034(11)       0.17438(10)       0.0000       0.25114(10)       0.14053(11)       0.14053(11)       0.10000       0.00000       0.00000(2)       0.00000(2)       0.0000(2)       0.00001(7)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7157(5) 0.714(4) 0.1155(3) 0.714(4) 0.1155(3) 0.750(8) U <sub>13</sub> 0.0022(3) 0.0040(4) 0.0041(5) 0.0062(2) 0.0032(7) 0.0033(7) 0.0013(7) 0.0044(10) 0.0066(7)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0114(2) 0.0119(4) 0.0119(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.0012(4) 0.0008(2) 0.0000(2) 0.000000
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(3) M(4) A O(1) O(2) O(2) O(1) O(2) O(3) O(1) O(2) O(3) O(4) O(2) O(1) O(2) O(2) O(3) O(2) O(3) O(2) O(3) O(4) O(2) O(1) O(2) O(3) O(2) O(3) O(4) O(2) O(3) O(2) O(3) O(4) O(2) O(3) O(2) O(3) O(4) O(5) O(1) O(2) O(2) O(3) O(2) O(3) O(4) O(2) O(3) O(4) O(2) O(3) O(2) O(3) O(4) O(2) O(3) O(2) O(3) O(2) O(3) O(4) O(2) O(3) O(4) O(2) O(3) O(2) O(3) O(2) O(3) O(4) O(2) O(3) O(4) O(7	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Na       0.73Na+0.27K       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       90H       U11       0.0062(4)       0.0075(7)       0.019(4)       0.603(2)       0.0075(7)       0.0152(15)       0.0182(15)       0.0182(15)       0.0182(9)       0.015(9)	U2 0.06Al+0.29Ti 0.03Cl U2 0.0069(4) 0.0069(4) 0.0069(4) 0.0065(5) 0.0113(5) 0.0059(4) 0.0065(5) 0.0113(5) 0.0059(4) 0.0065(10) 0.0124(9) 0.0119(13) 0.0094(9) 0.0119(13)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.10582(3) 0.3658(19) 0.35101(18) 0.36863(19) 0.35101(18) 0.335101(18) 0.3372(3) 0.189(5) U <sub>33</sub> 0.0069(4) 0.0070(4) 0.0062(6) 0.0117(6) 0.0109(4) 0.0099(9) 0.0141(13) 0.025(9) 0.01125(9) 0.01125(9)	y       0.06595(4)       0.17353(4)       0.08973(5)       0.17709(5)       0.0000       0.28089(4)       0.5000       0.28041(1)       0.17438(10)       0.0000       0.25114(10)       0.17170(11)       0.0000       U <sub>23</sub> 0.0000(2)       0.0000       0.0000       U <sub>23</sub> 0.0000(2)       0.0000       0.00014(7)       0.	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2765(5) 0.750(8) U <sub>13</sub> 0.0022(3) 0.0032(3) 0.0040(4) 0.0047(4) 0.0013(7) 0.0036(7) 0.0036(7)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0056(3) 0.111(2) 0.0119(4) 0.0119(4) 0.0112(4) 0.01122(4) 0.01122(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.0159(6) 0.0001(2) 0.0000(2) 0.0000(2) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000(7) 0.00009(7) 0.00003(7)
Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(3) M(4) A C(1) O(2) O(3) O(4) O(2) O(3) O(4) O(2) O(3) O(4) O(2) O(3) O(4) O(2) O(3) O(4) O(2) O(3) O(2) O(3) O(2) O(3) O(2) O(3) O(2) O(3) O(2) O(3) O(3) O(2) O(3) O(3) M(4) A (2) (3) (4) (5) (5) (6) (7) (7) (7) (7) (7) (7) (7) (7	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.81Mg+0.19Fe       1.97Ca+0.01Na       0.73Na+0.27K       40       40       40       40       40       40       20       1.90H       U1       0.0082(4)       0.0072(4)       0.0075(7)       0.019(5)       0.019(5)       0.015(2)       0.0055(10)       0.0075(7)       0.0076(9)       0.0135(9)       0.0135(9)       0.0115(9)       0.012(9)	U) ++0.86AI+0.29Ti ++0.02Mn 0.03Cl U₂ 0.0069(4) 0.0069(4) 0.0065(5) 0.0113(5) 0.0050(6) 0.0165(10) 0.0152(10) 0.0141(10) 0.0141(10) 0.0150(10)	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.1088(3) 0.36563(19) 0.35101(18) 0.36563(19) 0.35101(18) 0.3372(3) 0.36563(19) 0.35101(18) 0.3372(3) 0.3695(19) 0.3372(3) 0.3972(3) 0.3972(3) 0.3972(3) 0.3972(3) 0.3972(3) 0.3972(3) 0.3972(3) 0.0059(4) 0.0059(4) 0.0059(5)	y 0.06595(4) 0.17353(4) 0.08973(5) 0.0000 0.28089(4) 0.5000 0.28089(4) 0.5000 0.28934(11) 0.17438(10) 0.0000 0.25114(10) 0.14053(11) 0.11710(11) 0.0000 0.25114(10) 0.0000 0.25114(10) 0.0000 0.25114(10) 0.000000 0.0000 0.00000 0.00000 0.00000000	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.6125(3) 0.2766(5) 0.750(6) U <sub>15</sub> 0.0022(3) 0.0042(3) 0.0047(4) 0.0047(4) 0.0047(4) 0.0052(2) 0.0030(7) 0.0036(7) 0.0036(7)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0056(3) 0.111(2) 0.0119(4) 0.0101(4) 0.0112(4) 0.0112(4) 0.0122(4) 0.0122(4) 0.00122(4) 0.0001(1) <sup>4</sup> U <sub>12</sub> -0.0008(2) 0.0000(10) <sup>4</sup> U <sub>12</sub> -0.0008(2) 0.0000 0.000 0.000 0.000 0.000 0.0000 -0.0025(7) 0.00004(7) 0.0000(7) 0.0003(7) 0.0003(7)
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Site T(1) T(2) M(2) M(3) M(4) A (2/m) O(1) O(2) O(3) O(4) O(5) O(6) O(7) H T(1) T(2) M(1) M(2) M(3) M(4) A O(1) O(2) O(3) O(1) O(2) O(3) O(1) O(2) O(3) O(7) T(2) M(3) M(4) A O(1) O(2) O(3) O(1) O(2) O(3) O(7) T(2) M(3) M(4) A O(1) O(2) O(3) O(7) T(2) M(3) M(4) A O(1) O(2) O(3) O(7) T(2) M(3) M(4) A O(1) O(2) O(3) O(7) M(3) M(4) A O(1) O(2) O(7) M(3) M(3) M(4) A O(1) O(2) O(7) M(3) M(4) A O(1) O(2) O(7) M(3) M(4) A O(1) O(2) O(7) M(3) M(4) A O(1) O(2) O(7) M(3) M(4) O(7) M(3) M(4) O(7) M(3) M(4) O(7) O(7) M(3) M(4) O(7) O(7) M(3) M(4) O(7) O(7) M(3) M(4) O(7) O(7) O(7) M(3) M(4) O(7) O(7) M(3) M(4) O(7) O(7) M(3) O(7) O(7) O(7) M(3) O(7) O(7) M(3) O(7) O(7) M(3) O(7) O(7) M(3) O(7) O(7) O(7) M(3) O(7) O(7) O(7) M(3) O(7)	Occupancy (ap)       2.10Si+1.90Al       3.37Si+0.63Al       1.66Mg+0.34Fe       0.60Mg+0.25Fe       0.60Mg+0.25Fe       0.73Na+0.27K       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       40       20       1.90H       U1       0.0062(4)       0.0075(7)       0.019(4)       0.603(2)       0.0075(7)       0.0162(15)       0.0135(9)       0.015(9)       0.0115(9)       0.0115(9)       0.0115(13)	U) +++0.86Al+0.29Ti +++0.02Mn 0.03Cl 0.0069(4) 0.0069(4) 0.0069(4) 0.0065(5) 0.0113(5) 0.0013(5) 0.0059(4) 0.0065(10) 0.0124(9) 0.0119(13) 0.0094(9) 0.0141(10) 0.0149(14) Tameter.	x 0.27942(7) 0.29054(7) 0.0000 0.0000 0.0000 0.0000 0.10562(19) 0.11888(19) 0.35101(18) 0.3658(19) 0.35101(18) 0.36863(19) 0.35101(18) 0.335101(18) 0.3372(3) 0.189(5) U <sub>33</sub> 0.0069(4) 0.0070(4) 0.0069(4) 0.0069(4) 0.0069(4) 0.0099(9) 0.0117(6) 0.0099(9) 0.0192(14) 0.0192(14)	y       0.06595(4)       0.17353(4)       0.08973(5)       0.17709(5)       0.0000       0.28089(4)       0.5000       0.28041(1)       0.17438(10)       0.0000       0.25114(10)       0.17170(11)       0.17438(10)       0.0000       U23       0.0000(2)       0.0000       U23       0.0000(2)       0.0000(17)       0.00049(7)       0.00043(7)	z 0.30443(14) 0.81600(13) 0.5000 0.0000 0.5000 0.0000 0.2147(4) 0.7371(4) 0.7371(4) 0.7157(5) 0.7914(4) 0.1155(3) 0.6125(3) 0.2765(5) 0.750(8) U <sub>13</sub> 0.0022(3) 0.0032(3) 0.0040(4) 0.0047(4) 0.0013(7) 0.0062(2) 0.0036(7) 0.0036(7) 0.0036(7) 0.0036(7) 0.0006(10)	0.0066(3) 0.0066(3) 0.0074(3) 0.0113(3) 0.0056(3) 0.0113(3) 0.0056(3) 0.111(2) 0.0119(4) 0.0119(4) 0.0112(4) 0.0112(4) 0.01122(4) 0.0122(4) 0.0122(4) 0.0122(4) 0.01122(4) 0.01122(4) 0.01122(4) 0.0159(6) 0.0000(2) 0.0000(2) 0.0000(2) 0.0000(2) 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000(7) 0.000025(7) 0.00012(7) 0.00012(7) 0.0000

gaite" by Shimazaki *et al.* (1984), were characterized by their extremely high <sup>[4]</sup>Al (2.76-3.39 apfu) and K contents (0.62-0.75 apfu). Shimazaki *et al.* (1984) suggested that substantial replacement of Si by Al in the tetrahedral site might be crystallochemically necessary for the entry of K into the A site. However, relatively high <sup>[A]</sup>Na (0.70-0.92 apfu) and low K (0.09-0.28 apfu) contents in magnesiosadanagaite from the Kasuga-mura area are not consistent with their view. Figure 4 summarizes the relationships among K,  $X_{Fe^{2+}}$  [ = Fe<sup>2+</sup>/(Fe<sup>2+</sup> + Mg)] and <sup>[4]</sup>Al of calcic amphiboles with <sup>[4]</sup>Al > 2.5 apfu in this study and from the literature. The amphiboles with  $X_{Fe^{2+}} > 0.4$  show high K contents (0.30-0.84 apfu), whereas those with lower  $X_{Fe^{2+}}$  [< 0.3; this study, Mogessie *et al.* (1986) and Wang (1997)] do not show high K content (0.00-0.39 apfu) (Fig. 4). These chemical data indicate that high K substitution in the A site is not an essential feature for the Si-poor member of calcic amphiboles with low  $X_{Fe^{2+}}$ .

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Fig. 4. Relationship between K, <sup>[4]</sup>Al and  $X_{Fe^{2+}}$  contents of sadanagaite, potassicsadanagaite, magnesiosadanagaite, potassic-magnesiosadanagaite and potassic-ferrisadanagaite. The chemical data are from Banno *et al.* (this study), Hawthorne & Grundy (1977), Mogessie *et al.* (1986), Savel'eva & Korikovskii (1998), Sawaki (1989), Shimazaki *et al.* (1984), Sokolova *et al.* (2000), van Marcke de Lumen & Verkaeren (1985) and Wang *et al.* (1997). KFSAD, potassic-ferrisadanagaite.

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