1 **Mineralogical anatomy and implications of a Ti-Sc-rich ultrarefractory**
2 **inclusion from Sayh al Uhaymir 290 CH3 chondrite**

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Abstract

Titanium-rich minerals are common in Ca-Al-rich inclusions from primitive chondrites. They are important not only for testing the condensation models for a gas with a solar composition, but also for constraining the redox conditions of the early solar nebula. In this study, we report the detailed mineralogical features and its oxygen isotope compositions of a Ti-Sc-rich **ultrarefractory** inclusion A0031 from a CH3 chondrite Sayh al Uhaymir 290. The A0031 inclusion has a compact and layered texture with the interior consisting of panguite, Sc-rich anosovite, Ti-rich davisite, and anorthite. A few hexaferrum, perovskite, and spinel crystals are present as inclusions in these minerals. Outside of Ti-rich davisite are a layer of Al-Ti-rich diopside and two grains of enstatite. This texture strongly suggests that A0031 has a condensation origin. Panguite is its third occurrence in nature and similar in composition to the type panguite from the Allende meteorite. Sc-rich anosovite in A0031 has a chemical formula of $(\text{Ti}^{4+}, \text{Ti}^{3+}, \text{Mg}, \text{Sc}, \text{Al})_3\text{O}_5$ with the pseudobrookite structure. This is the second report of Ti_3O_5 in nature, but is the first description of anosovite formed in the solar nebula as an **ultrarefractory** phase. The discovery of Sc-rich anosovite in A0031 reveals the stability of Ti_3O_5 in the early solar nebula and supports the prediction of previous equilibrium condensation calculations. The panguite, Sc-rich anosovite, and Ti-rich davisite in A0031 show a large variation in $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$. The primitive nature of A0031 implies that the variations in $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ among different Ti-rich minerals are primary features. We propose that the distribution of Ti^{3+} and Ti^{4+} could be controlled mainly by their various competition abilities of incorporating into these Ti-Sc-Al-rich minerals. Similarity of $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ value between Ti-rich davisite from A0031 and those in other carbonaceous chondrites indicates that most refractory inclusions might have formed in highly reducing nebular settings. **The ^{16}O -depleted isotope compositions of A0031 confirm the existence of diverse oxygen reservoirs for CH Ca-Al-rich inclusions in the solar nebula.**

1. INTRODUCTION

Calcium-Aluminum-rich inclusions (CAIs) in primitive chondrites are mainly composed of aggregates of oxides and silicates of calcium and aluminum (Brearley and Jones, 1998; MacPherson, 2003), which have high condensation temperatures (Grossman, 1972; Lodders, 2003). The constituent minerals in CAIs are similar to the early phases that could have condensed out of a gas of solar composition predicted by thermodynamic calculations (Grossman, 1972; Yoneda and Grossman, 1995; Ebel and Grossman, 2000; Petaev and Wood, 2000; Ebel, 2006). This similarity indicates that CAIs in primitive chondrites were the first solids formed in the early solar nebula. Such an inference is well supported by the extremely old ages of pristine CAIs (~4567 Ma, Amelin et al., 2002; Bouvier and Wadhwa, 2010; Connelly et al., 2012). Therefore, primitive refractory minerals observed in CAIs may provide crucial clues to constraining the physicochemical conditions and processes in the early solar nebula (MacPherson, 2003).

Titanium is a refractory element during the condensation of high-temperature gases (Lodders, 2003). Based on the available data from condensation calculations for a gas with a solar composition, Ti can form individual oxides (e.g., Ti_2O_3 , Ti_3O_5 , Ti_4O_7 , and TiO_2) and Ca-titanates (e.g., CaTiO_3 , $\text{Ca}_4\text{Ti}_3\text{O}_{10}$, and $\text{Ca}_3\text{Ti}_2\text{O}_7$) (e.g., Lodders, 2003; Ebel, 2006). However, the most common Ti-rich and Ti-bearing minerals in refractory inclusions from primitive chondrites are perovskite, Ca-clinopyroxene (grossmanite, Ma and Rossman, 2009a; Ti-rich davisite, Ma and Rossman, 2009b; Ti-rich kushiroite, Kimura et al., 2009; Ti-rich diopside), and hibonite. Less common Ti-rich minerals observed in CAIs include panguite ($(\text{Ti}^{4+}, \text{Sc}, \text{Al}, \text{Mg}, \text{Zr}, \text{Ca})_{1.8}\text{O}_3$, Ma et al., 2012), kangite (Ma et al., 2013), and possible Ti_4O_7 -type oxide (Haggerty, 1978). Besides these Ti-rich minerals observed in CAIs, a few pure Ti-oxide minerals have also been described in matrix and chondrules, e.g., Ti_3O_5 (Brearley, 1993), rutile (TiO_2 , Ma and Rossman, 2009c), and tistarite (Ti_2O_3 , Ma and Rossman, 2009c). Their exact origins and formation processes remain not well constrained, although some of these Ti-oxide minerals probably formed in the early solar nebula. For

example, Ti_3O_5 grains were identified in the matrix of a chondrite clast in the Nilpena polymict ureilite and are nano-sized (Brearley, 1993). A presolar origin for these tiny Ti_3O_5 grains cannot be excluded based on the current data (Brearley, 1993). In summary, no $\text{Ca}_4\text{Ti}_3\text{O}_{10}$, $\text{Ca}_3\text{Ti}_2\text{O}_7$, and Ti_3O_5 firmly condensed from the solar nebula have been found in chondrites yet. Finding these high-Ti phases in CAIs from primitive chondrites is important for constraining the processes that have prevailed in the early solar nebula and for evaluating the reliability of theoretical models, especially that Ti_3O_5 was predicted to be a stable Ti-oxide by many equilibrium condensation models when Ti was considered (Grossman, 1972; Yoneda and Grossman, 1995; Ebel and Grossman, 2000; Petaev and Wood, 2000; Ebel, 2006).

Distinct from other major elements (e.g., Al, Ca, Mg, and Si) in CAIs, titanium may have various oxidation states Ti^{3+} and Ti^{4+} . This unique feature makes it possible that Ti-minerals might be used as proxies of oxygen fugacity in the early solar nebula (e.g., Beckett et al., 1988; Simon et al., 1991, 2007; Dyl et al., 2011; Ma et al., 2012). In the literature, the majority of investigations on oxidation states of Ti in CAIs mainly focus on pyroxene (Dowty and Clark, 1973; Simon et al., 1991, 2007; Grossman et al., 2008; Dyl et al., 2011) and hibonite (Beckett et al., 1988; Giannini et al., 2011; Doyle et al., 2014). The most important discovery about Ti in CAIs is the presence of Ti^{3+} in pyroxene and hibonite, which strongly supports that CAIs have been formed in highly reducing solar nebular conditions. By comparing with crystallization experiments under controlled oxygen fugacity conditions, Grossman et al. (2008) proposed that Ti^{3+} -bearing Ca-clinopyroxene + melilite pairs in natural refractory inclusions might have crystallized at $\log f\text{O}_2 = -19.8 \pm 0.9$, if they crystallized at ~ 1509 K. Previous investigators also noticed that a Ti-rich/bearing mineral might have various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values at different stages within a single CAI or different Ti-rich/bearing minerals within a single CAI may also have various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values (e.g., Simon et al., 1991, 2006, 2007; Dyl et al., 2001; Ma et al., 2012). However, whether all the variations in $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values within a single Ti-rich/bearing mineral and between different minerals within a single CAI reflect a change of oxygen fugacity in the early solar nebula is still an open question (e.g.,

Dyl et al., 2011; Simon et al., 2012; Young et al., 2012; Ma et al., 2012, 2013). It deserves more investigations on natural CAIs in primitive chondrites and their analogues in synthetic experiments (e.g., Grossman et al., 2008; Paque et al., 2013; Doyle et al., 2014).

Zhang and Hsu (2009) observed a Ti-Sc-rich CAI (designated A0031) containing a few fine-grained Ti-Sc-rich minerals from a CH3 chondrite Sayh al Uhaymir (SaU) 290. Recently, we performed further detailed chemical, structural, and oxygen isotope studies on these fine-grained Ti-rich minerals and observed two rare Ti-rich oxide minerals (Zhang et al., 2014b). One is panguite, an orthorhombic Sc-rich titania mineral (Ma et al., 2012); the other is anosovite, a Sc-rich titania with a pseudobrookite structure. The latter is different in crystal structure and chemistry from the known Ti-Sc-rich oxides in primitive chondrites (Rubin, 1997) and represents a new Ti-rich refractory mineral formed in the solar nebula. Here, we report the detailed mineralogical and isotope features of this Ti-Sc-rich CAI (A0031) and discuss their implications for solar nebula processes.

2. ANALYTICAL METHODS

Petrographic textures of the CAI A0031 were observed by using a Zeiss 1550VP Field Emission scanning electron microscope (FE-SEM) with backscattered electron (BSE) mode at California Institute of Technology (Caltech) and a JSM 7000F FE-SEM at Hokkaido University. A 2-nA electron beam, accelerated at a voltage of 15 kV, was used. Semi-quantitative compositional analyses for fine-grained minerals and X-ray elemental mapping were also performed with an energy dispersive spectroscopic detector (EDS) attached on the JSM 7000F FE-SEM.

Quantitative chemical analyses of oxide and silicate minerals in this study were conducted with a JEOL 8200 electron microprobe with Wavelength Dispersive Spectrometer (WDS) mode at Caltech. The machine was operated under an accelerating voltage of 10 or 15 kV and a focused beam of 5 or 10 nA. Standards for the analysis were anorthite (CaK α , AlK α , SiK α), TiO₂ (TiK α), synthetic forsterite (MgK α), V₂O₅ (VK α), ScPO₄ (ScK α), zircon (ZrL α),

synthetic fayalite ($\text{FeK}\alpha$), and Cr_2O_3 ($\text{CrK}\alpha$). Analyses were processed with the CITZAF correction procedure (Armstrong, 1995). The detection limits are 0.04 wt% for Sc, 0.13 wt% for Zr, 0.04 wt% for Ca, 0.05 wt% for Ti, 0.04 wt% Al, 0.06 wt% for Fe, 0.02 wt% for V, 0.06 wt% for Cr, 0.03 wt% for Mg, 0.04 wt% for Si, and 0.29 wt% for Y. The concentrations of Ti^{3+} in Ti-rich pyroxene, panguite, and anosovite were calculated based on their stoichiometry (4 cations and 6 oxygen atoms for pyroxene; 1.8 cations and 3 oxygen atoms for panguite; and 3 cations and 5 oxygen atoms for anosovite), assuming titanium is the only element with various valence states in these minerals.

Electron backscatter diffraction (EBSD) analyses at a submicrometer scale were carried out to determine the crystal structure of fine-grained minerals in A0031, especially the two rare Ti,Sc-rich oxides. The measurements were performed on the vibro-polished section using the methods described in Ma and Rossman (2008, 2009a). An HKL EBSD system on the Zeiss FE-SEM mentioned above was used for these measurements and operated at 20 kV and 6 nA in a focused beam configuration with a 70° tilted stage and variable pressure (20 Pa) mode. The EBSD system was calibrated using a single-crystal silicon standard. The experimental EBSD patterns of the two Ti-dominant oxides were indexed with the structures of synthetic Ti_2O_3 (Newnham and de Haan, 1962; Vincent et al. 1980; Rice and Robinson 1977), synthetic Ti_3O_5 (Onoda 1998), Sc_2TiO_5 (Ito, 1971), TiO (Loehman et al. 1969), TiO_2 (anatase, rutile, and brookite) reported in Ballirano and Caminiti (2001), Howard et al. (1992), and Meagher and Lager (1979), synthetic Ti_4O_7 (Marezio and Dernier, 1971), and the newly defined minerals panguite and kangite (Ma et al. 2012; 2013). The HKL software automatically suggests indexing solutions ranked by the lowest “mean angular deviation” (MAD) as an index of “goodness of fit.” MAD numbers <1 are considered desirable for accurate solutions.

To determine the distribution of oxygen isotopes within A0031, we performed oxygen isotope mapping with the isotope microscope system consisting of a Cameca IMS-1270 SIMS instrument and a high-efficiency Stacked CMOS-type Active Pixel Sensor (SCAPS) ion

imager at Hokkaido University (Takayanagi et al., 1999; Yurimoto et al., 2003; Sakamoto et al., 2008). This isotopic microscope system has been widely used to reveal isotopic variations in extraterrestrial materials (e.g., Nagashima et al., 2004; Sakamoto et al., 2007; Park et al., 2012; Hashiguchi et al., 2013). The analytical procedure in this study is generally similar to that in Park et al. (2012) except for that a primary beam current of ~2 nA was used in this study. Four measurement cycles were performed to obtain secondary ion images of ^{16}O and ^{18}O . Each cycle contains 2 frames for ^{16}O and 100 frames for ^{18}O with each frame of 5 seconds. Before and after the oxygen isotope mapping, ^{27}Al and ^{28}Si were also mapped for 3-5 frames with each frame of 5 seconds to better constrain the locations of minerals in A0031. The $\delta^{18}\text{O}$ isotopograph of A0031 was obtained by calculating the secondary ion ratios of $^{18}\text{O}/^{16}\text{O}$ for each pixel and then calibrated with a forsterite grain closely nearby, whose oxygen isotopic composition was determined by spot analysis using the same SIMS instrument. To reduce random noises caused by the statistical fluctuation of secondary ions, image smoothing with an average of 5×5 pixels was applied.

3. RESULTS

3.1. Petrographic description of SaU 290

SaU 290 is a typical CH chondrite, similar in texture and mineralogy to other CH chondrites, e.g., ALH 85085 and NWA 739 (Grossman et al., 1989; Kimura et al., 1993; Krot et al., 2006; Zhang and Hsu, 2009). It consists of abundant small type I chondrules and refractory inclusions; their sizes are usually less than 100 μm . Cryptocrystalline chondrules and glassy chondrules are common in this chondrite. A few metal grains in SaU 290 have been partially weathered. However, silicate minerals in chondrules and mineral fragments remain intact, indicating that no silicate minerals were affected by terrestrial weathering.

3.2. Petrography and mineral assemblage of A0031

The CAI A0031 observed in the CH3 chondrite SaU 290 is ~25 μm across. It has a

compact and layered texture with an irregular shape (Fig. 1). The original CAI could be slightly larger than it appears now, since the dark rim of A0031 in Fig. 1 appears truncated. The central part of A0031 consists mainly of panguite (~23 vol%) and davisite (~40 vol%), with the former enclosed by the latter (Fig. 1). The panguite grains are 1-4 μm in length and subhedral in shape. Some of them connect with each other and form irregular aggregates. Two subhedral anosovite grains are closely associated with panguite aggregates. Each of the two grains of anosovite is about 1.5 μm in size. The shape of panguite is confining to those of anosovite grains (Fig. 2). Three small anorthite grains (1-2 μm in size) are also in close contact with panguite. Minor minerals hexaferrum, perovskite, and spinel mainly occur as mineral inclusions in A0031. The grain sizes of hexaferrum grains vary from ~100 nm to 2 μm . They are included in panguite, davisite, and anosovite. Spinel grains are submicron in size and included in both davisite and anorthite (Fig. 3). Only one perovskite grain was identified based on its high Ti and Ca concentrations in elemental maps (Fig. 3). It is ~500 nm in size and included in panguite. Surrounding davisite, there is an Al-Ti-rich diopside rim (~30 vol%), which is about 1-2 μm thick. Outside of the Al-Ti-rich diopside rim, two separated anhedral-subhedral enstatite grains (<2 μm in size) are also observed (Fig. 1).

3.3. Crystal structure and chemistry of minerals in A0031

Due to small grain sizes of most constituent minerals in A0031, only relatively large minerals (hexaferrum, davisite, Al-Ti-rich diopside, panguite, and anosovite) were determined for quantitative compositions in this study.

Chemical compositions of two relatively large hexaferrum grains (1-2 μm in size) in A0031 were determined by EDS and the results indicate that hexaferrum is dominated by Fe, Ir, Mo, and Os with a decreasing sequence of mole percent. The two grains of hexaferrum show a large chemical variation from each other ($\text{Fe}_{62}\text{Ir}_{19}\text{Mo}_{12}\text{Os}_7$ and $\text{Fe}_{48}\text{Ir}_{28}\text{Mo}_{17}\text{Os}_7$, respectively).

Five spot analyses were performed on different parts of davisite in A0031. The EPMA

results (Table 1) show that davisite contains high and varying Al_2O_3 (18.1-19.4 wt%), Sc_2O_3 (8.3-10.3 wt%), and $\text{TiO}_2+\text{Ti}_2\text{O}_3$ (8.11-11.4 wt%). Based on the stoichiometry of davisite, the five spot analyses have variable $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values (0.52-0.71) with an average of 0.63. It is noteworthy that the davisite grains contain 1.13-1.89 wt% ZrO_2 , 0.80-1.03 wt% V_2O_3 , 0.60-1.01 wt% Y_2O_3 . Four spot analyses were performed on Al-Ti-rich diopside in A0031. Compared with davisite in A0031, Al-Ti-rich diopside contains much lower Al_2O_3 , Sc_2O_3 , and TiO_2 . The contents of ZrO_2 , V_2O_3 , and Y_2O_3 in Al-Ti-rich diopside are also lower than those in davisite (Table 1). No quantitative EPMA analysis was performed on the two grains of enstatite outside of the Al-Ti-rich diopside rim. The EDS results (performed at 15 kV) show that the enstatite grains contain minor Al_2O_3 , Sc_2O_3 , and TiO_2 , which could be due to contamination from surrounding Al-Ti-rich diopside.

Panguite and anosovite are rare phases in refractory inclusions. Their crystal structures are determined with the EBSD technique. Both panguite and anosovite have a well-defined experimental EBSD pattern (Figs. 4-5). The EBSD pattern (Fig. 4a) of panguite in A0031 is almost identical to that reported in Ma et al. (2012). The indexing result (Fig. 4b) based on the unit cell data for panguite from the Allende meteorite (Ma et al. 2012) gave a best fit with a mean angular deviation of 0.42° , indicating that the panguite grains in A0031 also have an orthorhombic *Pbca* structure. Three spot EPMA analyses were performed on different panguite grains in A0031. The EPMA results show almost identical chemical compositions. Similar to the type panguite from Allende (Ma et al., 2012), panguite in A0031 contains high Sc_2O_3 , Al_2O_3 , Y_2O_3 , and ZrO_2 with an average of 14.42 wt%, 8.76 wt%, 4.59 wt%, and 4.51 wt%, respectively (Table 2). According to the stoichiometry of panguite, panguite in A0031 has an empirical formula of $(\text{Ti}^{4+}_{0.79}\text{Sc}_{0.27}\text{Al}_{0.23}\text{Mg}_{0.15}\text{Ti}^{3+}_{0.06}\text{Y}_{0.05}\text{Zr}_{0.04}\text{Cr}_{0.04}\text{Si}_{0.03}\text{V}_{0.03})_{\Sigma=1.80}\text{O}_3$, based on its average composition. The $\text{Ti}^{3+}/\text{Ti}^{(\text{tot})}$ value is 0.07, also similar to that of the type panguite from the Allende meteorite (Ma et al., 2012).

The EBSD pattern of anosovite was matched with those of rutile, tistarite (Ti_2O_3), panguite, pseudobrookite, armalcolite, Sc_2TiO_5 , and Ti_3O_5 structures. However, it can be

indexed only by the pseudobrookite-type structure to give a best fit based on the unit cell data for synthetic Ti_3O_5 (Onoda, 1999) (Fig. 5b), with a mean angular deviation of 0.31° . This fitting result indicates that anosovite in A0031 is an orthorhombic mineral in space group *Cmcm*. The two grains of anosovite in A0031 have compositions distinctly different from those of panguite (Table 2). Compared with panguite, anosovite in A0031 contains much high $\text{TiO}_2(\text{tot})$ (>70 wt%; Fig. 6). Meanwhile, the contents of Al_2O_3 , Y_2O_3 , and ZrO_2 in anosovite are lower than those in panguite (Table 2; Fig. 6). Based on the stoichiometry for a pseudobrookite-structure phase, the two anosovite grains in A0031 have empirical formula of $(\text{Ti}^{4+}_{1.37}\text{Ti}^{3+}_{0.64}\text{Mg}_{0.35}\text{Sc}_{0.26}\text{Al}_{0.19}\text{V}_{0.05}\text{Ca}_{0.04}\text{Si}_{0.03}\text{Fe}_{0.03}\text{Cr}_{0.03}\text{Zr}_{0.02})_{\Sigma=3.00}\text{O}_5$ and $(\text{Ti}^{4+}_{1.35}\text{Ti}^{3+}_{0.53}\text{Mg}_{0.33}\text{Sc}_{0.31}\text{Al}_{0.22}\text{Ca}_{0.06}\text{V}_{0.05}\text{Si}_{0.04}\text{Fe}_{0.03}\text{Cr}_{0.03}\text{Zr}_{0.04}\text{Y}_{0.02})_{\Sigma=3.00}\text{O}_5$, respectively. Their $\text{Ti}^{3+}/\text{Ti}^{(\text{tot})}$ values are 0.32 and 0.28, respectively. The generalized chemical formula of the anosovite is $(\text{Ti}^{4+}, \text{Ti}^{3+}, \text{Mg}, \text{Sc}, \text{Al})_3\text{O}_5$. The calculated X-ray powder diffraction data (in Å for $\text{CuK}\alpha 1$) for anosovite are given in Table 3, using the synthetic Ti_3O_5 unit cell and atom coordinates from Onoda (1999), and the empirical formula of this study, using PowderCell 2.4.

3.4. SCAPS oxygen isotope compositions of A0031

The SCAPS oxygen isotope mapping result (Fig. 7) shows that minerals in A0031 appear to have almost identical oxygen isotope compositions except for the rim of A0031. Panguite grains have an average $\delta^{18}\text{O}$ value of -9.4 ± 2.5 ‰; while davisite grains have an average $\delta^{18}\text{O}$ value of -9.2 ± 1.7 ‰. No hot spots of $\delta^{18}\text{O}$ value are observed in A0031. The thin high- $\delta^{18}\text{O}$ rim in Fig. 7 is probably caused by a large variation of oxygen concentration at the margin of A0031 (complex terrestrial weathering products occur along boundary between A0031 and surrounding components) during SCAPS sputtering (Fig. 1). However, we cannot totally exclude the possibility that the rim is enriched in $\delta^{18}\text{O}$ than the interior of A0031.

4. DISCUSSION

4.1. Anosovite, Ti-, Sc-rich pseudobrookite-structure phase: A new refractory mineral

Pseudobrookite-structure phases have an ideal chemical formula A_2BO_5 , where A octahedral sites are occupied by +3 valence cations and B octahedral sites are occupied by +4 valence cations. In this study, due to the small grain size and complex compositions of anosovite in A0031, we were not able to determine cation site occupancies. If the anosovite grains in A0031 have an ordered distribution of cations at the two octahedral sites with the B octahedral site occupied only by Ti^{4+} , the chemical formula of the anosovite in A0031 would be $(Ti^{3+}, Sc, Al, Ti^{4+}, Mg)_2 Ti^{4+} O_5$ based on the dominant valency rule (Hatert and Burke, 2008). This chemical formula is corresponding to an end member of $Ti^{3+}_2 Ti^{4+} O_5$. In this case, Sc and Al substitute Ti^{3+} at the A sites by $(Sc, Al) \leftrightarrow Ti^{3+}$; whereas Ti^{4+} and Mg incorporate into the A sites by the substitution $Ti^{4+} + Mg \leftrightarrow 2(Ti^{3+}, Sc, Al)$.

For the case of disordered distribution of cations at A and B octahedral sites, if the distribution of cations are highly disordered (e.g., >37%) at the two octahedral sites in the pseudobrookite structure, the chemical formula of the anosovite in A0031 is $(Ti^{4+}, Ti^{3+}, Mg, Sc, Al)_3 O_5$, also corresponding to an end member of $Ti_3 O_5$. Previous investigations have found that the order-disorder distributions of cations in the pseudobrookite structure are strongly temperature-dependent with higher cation disordering for higher temperatures (Navrotsky, 1975; Kolitsch and Tillmanns, 2003). At high temperatures, Ti^{4+} has a high preference for the more distorted A site in pseudobrookite-structured A_2BO_5 compounds. For example, at high temperatures (1123–1423 K), synthetic Sc_2TiO_5 shows a structure formula $(Sc_{0.6}Ti_{0.4})_2(Sc_{0.8}Ti_{0.2})O_5$ (Kolitsch and Tillmanns, 2003). Since A0031 is a Ti-Sc-rich refractory inclusion, its constituent minerals including anosovite should have formed at a high-temperature condition. Thus, in this study, we favor that the anosovite grains in A0031 have a highly disordered structure and have a chemical formula $(Ti^{4+}, Ti^{3+}, Mg, Sc, Al)_3 O_5$ with a simplified formula $Ti_3 O_5$, although its exact order-disorder degree of cations is unclear.

Anosovite observed in A0031 is the second occurrence of $Ti_3 O_5$ in nature. The first natural occurrence of $Ti_3 O_5$ with a pseudobrookite structure was reported in a CI-like

286 carbonaceous chondrite clast in the Nilpena polymict ureilite (Brearley, 1993). It was
 287 identified by transmission electron microscopy and selected area electron diffraction.
 288 However, there are a few distinctions between the anosovite in A0031 and the Ti_3O_5 phase in
 289 Nilpena ureilite. The first distinction is their occurrences. The Ti_3O_5 grains in Nilpena ureilite
 290 occur as clusters or isolated grains in a matrix of Si-rich amorphous material, phyllosilicates,
 291 sulfides, and oxides (Brearley, 1993). Based on this occurrence, its exact origin and genetic
 292 relationships with surrounding fine-grained phases are still not well known. However, the
 293 anosovite grains **in this study** are located in a CAI and closely associated with panguite and
 294 davisite, indicating its solar origin. The second distinction is their chemical compositions. The
 295 Ti_3O_5 grains in Nilpena ureilite appear as a pure Ti-oxide and no other elements were detected
 296 (Brearley, 1993). In contrast, the anosovite grains in A0031 have high concentrations of Sc, Al,
 297 and Zr, similar to the associated panguite and davisite. This chemical similarity also supports
 298 the solar origin for anosovite in A0031, rather than **presolar** grains included in a CAI. The
 299 third distinction is their grain sizes although both are fine-grained. The Ti_3O_5 grains in
 300 Nilpena ureilite range from 0.05–0.25 μm in diameter (Brearley, 1993); however, the
 301 anosovite grains in A0031 are 1–1.5 μm in diameter. Thus, the anosovite in A0031 is a new
 302 and unique Ti-rich oxide firmly formed in the solar nebula. The lack of oxygen isotopic
 303 anomaly in the anosovite in A0031 based on our SCAPS data also supports this conclusion.
 304 The pseudobrookite-structure mineral anosovite $(\text{Ti}^{4+}, \text{Ti}^{3+}, \text{Mg}, \text{Sc}, \text{Al})_3\text{O}_5$ in A0031 joins
 305 various Ti-, Zr-, Y-, and Sc-rich oxides and silicates that have been observed in refractory
 306 inclusions from carbonaceous chondrites, including allendeite, tazheranite, zirconolite,
 307 panguite, thortveitite, lakargiite, eringaite, grossmanite, davisite, and kangite (Allen et al.,
 308 1980; Hinton et al., 1988; El Goresy et al., 2002; Ma and Rossman, 2008b, 2009b; Ma, 2011,
 309 2012; Ma et al., 2011, 2012, 2013, 2014). However, different from other Ti-, Zr-, Y-, and
 310 Sc-rich oxide and silicates, the presence of anosovite $(\text{Ti}^{4+}, \text{Ti}^{3+}, \text{Mg}, \text{Sc}, \text{Al})_3\text{O}_5$ in A0031 for
 311 the first time confirms the stability of Ti_3O_5 in the early solar system, which was predicted in
 312 previous equilibrium condensation models (Yoneda and Grossman, 1995; Ebel and Grossman,

2000; Petaev and Wood, 2000).

4.2. Condensation origin of the CAI A0031 in a ¹⁶O-poor nebular setting

Our mineral chemistry data indicate that Ti-rich minerals (perovskite, panguite, anosovite and davisite) in A0031 have various $\text{Ti}^{3+}/\text{Ti}^{(\text{tot})}$ values. This feature is closely related to the origin of A0031. Therefore, understanding the origin of A0031 is crucial to interpret the significance of various $\text{Ti}^{3+}/\text{Ti}^{(\text{tot})}$ values for different Ti-rich minerals in A0031.

Generally, two major origins have been proposed to explain the formation of CAIs in SaU 290 (Zhang and Hsu, 2009). One group of CAIs in SaU 290 could be direct gas-solid condensates from the solar nebula. They usually have irregular shapes and layered textures. The other group of CAIs might have crystallized from Ca-Al-rich refractory melt droplets or experienced subsequent melting and **recrystallization**. They usually have rounded shapes and a texture typical of igneous origin. The petrographic texture and mineralogy of A0031 imply that it might have a condensation origin. The first evidence is the irregular shape of A0031 and its layered texture. An igneous origin cannot account for the layered texture of A0031. The second evidence would be the crystallization sequence of minerals in A0031, which is generally consistent with the formation sequence of refractory phases based on theoretical calculation of a solar-composition gas (Ebel, 2006). Based on the petrographic texture, the formation of constituent minerals in A0031 can be grouped into four major stages. (1) The first stage is the formation of hexaferrum, perovskite, and spinel; all these phases occur as inclusions in other minerals. (2) The second stage is the formation of davisite, anosovite, panguite, and anorthite. The connection between different panguite grains and between panguite and anosovite is generally consistent with collisional aggregation of particles in the early solar nebula. However, the formation of anosovite might be slightly earlier than that of panguite since the shape of panguite is confining to that of anosovite (Fig. 2). The duration for davisite formation might be longer than those for panguite and **anosovite** since the latter two minerals are enclosed by davisite. The third (3) and forth (4) stages are corresponding to the formation of Al-, Ti-rich diopside rim and enstatite, respectively. **Since the Al-, Ti-rich**

diopside contains distinctly lower Al_2O_3 and TiO_2 compared with Ti-rich davisite and enstatite is a typical chondrule mineral and is also very rare in amoeboid olivine aggregates (Krot et al., 2004), their formations may not be related to condensation in the region where the majority of refractory inclusions from CH chondrites formed. It is likely that the Al-, Ti-rich diopside rim and enstatite within A0031 have formed in a less refractory setting, such as chondrule-forming setting/region. In theoretical models that Ti was included (e.g., Yoneda & Grossman, 1995; Ebel & Grossman, 2000; Petaev & Wood, 2000), perovskite and spinel are always earlier condensates with higher condensation temperatures than those for Ca-pyroxene and feldspar, which are in turn higher than that for orthopyroxene. The difference of formation sequence between constituent minerals in A0031 and those in theoretical models could be due to the complex chemical compositions. For example, the high concentrations of Ir, Mo, and Os indicate that the Fe-rich alloy grains in A0031 are more refractory and have higher condensation temperatures than pure Fe-metal. Thermodynamic calculation by Ma et al. (2014) revealed that hexaferrum with Fe as the dominant element in mole might be stable at a temperature of >1400 K, although the reason why Ni is almost absent in hexaferrum based on the EDS result remains unknown. It is likely that Ni is enriched in other metal alloys but depleted in hexaferrum or hexamolybdenum. For example, Ma et al. (2014) observed the coexistence of Ni-Fe-Ir-Ru alloy and hexamolybdenum ($\text{Mo}_{0.258}\text{Fe}_{0.255}\text{Ru}_{0.231}\text{Os}_{0.109}\text{Ir}_{0.094}\text{Ni}_{0.027}\text{W}_{0.020}\text{Re}_{0.006}$) in a fine-grained refractory inclusion from USNM polished thin section 3509HC12. The presence of Sc may also enhance the condensation temperature of anosovite; while the presence of Sc, Ti, and Al might lead to a much higher condensation temperature of Ti-rich davisite than Ca-pyroxene. Assuming that A0031 was formed at a total pressure of $\sim 10^{-4}$ bar (Meibom et al., 1999), the temperature interval for the formation of A0031 might be >1400 K to ~ 1300 K based on the presence of perovskite, spinel, and orthopyroxene (Ebel, 2006).

Petrographic observations in this study indicate that A0031 has a very high abundance of two Sc-, Zr-, Y-rich **ultrarefractory** phases, panguite and davisite. Especially, the abundance of

panguite in A0031 is up to ~20 vol%; this is the highest abundance of panguite in CAIs up to date, compared with those observed in Allende and Murchison (Ma et al., 2011, 2012). This mineral assemblage implies that A0031 is an **ultrarefractory** inclusion in the CH chondrite SaU 290. This inference is supported by the bulk enrichment of refractory lithophile elements, although the concentrations of rare-earth elements in A0031 were not determined because of the small grain size. Given the average compositions for the oxide and silicate minerals in A0031 and their apparent abundances, we calculated the bulk composition of oxide and silicate portion in A0031. The result reveals a high enrichment of refractory lithophile elements Sc (9500), Y (8000), Zr (3500), Ti (260), Ca (13), and Al (7), relative to those for CI chondrites (Anders and Grevesse, 1989). Based on the geochemical and cosmochemical similarity between Y and heavy rare-earth elements (HREE) (e.g., El Goresy et al., 2002; Ma et al., 2013), it is likely that the CAI A0031 is also enriched in HREE, which is a characteristic feature of **ultrarefractory** inclusions.

Oxygen isotopic compositions of CAIs in primitive chondrites have been widely used to constrain their reservoirs in the solar nebula (e.g., Yurimoto et al., 2008). However, pristine CAIs in most carbonaceous chondrites, enstatite chondrites, and unequilibrated ordinary chondrites are highly ^{16}O -enriched (Yurimoto et al., 2008; Krot et al., 2012); whereas some CAIs in CH chondrites and those in CB are ^{16}O -depleted (Sahijpal et al., 1999; Kobayashi et al., 2003; Krot et al., 2012, 2015). Krot et al. (2012) observed that most of these ^{16}O -depleted CAIs have igneous textures and are less refractory (without hibonite and grossite). Based on these observations, they suggested that most of these ^{16}O -depleted CAIs may have resulted from complete melting of pre-existing ^{16}O -enriched or ^{16}O -depleted CAIs in ^{16}O -poor gas-melt plume (Krot et al., 2012). However, detailed oxygen isotope measurements of incompletely melted CAIs within porphyritic chondrules or with igneous rims in CH chondrites show little evidence for O-isotope exchange between relict CAIs and the host chondrule melts (Krot et al., 2015). This observation is well consistent with the sluggish O diffusion in solid minerals (e.g., spinel and pyroxene) during chondrule formation (Ryerson

and McKeegan, 1994; Zhang et al., 2014a). In this study, the $\delta^{18}\text{O}$ -values ($\sim -9\text{‰}$) of minerals in the interior of A0031 are similar to those of ^{16}O -depleted CAIs in CH chondrites (Krot et al., 2012, 2015). However, as discussed above, A0031, at least the majority of A0031, has a condensation origin. This may imply that its ^{16}O -depleted isotopic compositions of A0031 is a primitive feature, rather than due to O-isotope exchange during formation of the Al-, Ti-rich diopside rim and enstatite. Thus, our oxygen isotope data of A0031 confirm that the CH CAIs have at least two oxygen reservoirs in the solar nebula, consistent with the inference by Yurimoto et al. (2008).

4.3. Origin of various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values for coexisting Ti-rich minerals

Our data show that the closely coexisting panguite, anosovite, and Ti-rich davisite in A0031 have a large variation in $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ value from 0.07 to 0.63. This large variation cannot be accounted for by possible large uncertainties of the method (c.f., Simon et al., 2012). Various Ti valence states for closely coexisting Ti-rich minerals have been reported in the literature (e.g., Ma et al., 2012, 2013). Basically, three possibilities could be considered to interpret the varying $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values between panguite, anosovite, and Ti-rich davisite in A0031. 1) All three Ti-rich minerals in A0031 formed under a reducing nebular condition, but experienced a secondary oxidization event in the nebula or on the parent bodies (c.f., Ma et al., 2013) that resulted in a change in $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ to various extents for different minerals. 2) The various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values between panguite, anosovite, and Ti-rich davisite are primary features with different minerals formed under various redox conditions and then mixed with each other (c.f., Ma et al., 2012). 3) The various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values between different Ti-rich minerals are also primary features. They formed under a reducing condition but the distribution of Ti^{3+} and Ti^{4+} are mainly controlled by their various competition abilities of incorporating into these Ti-Sc-Al-rich minerals.

Ma et al. (2013) discovered a new Sc-Ti-rich oxide, kangite, in an **ultrarefractory** inclusion from Allende, where kangite is closely coexisting with davisite and they have a large difference in $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$. They interpreted that kangite with a low $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ value formed

through low-temperature oxidation of an Sc-Ti³⁺-rich oxide when they excluded the possibility of a primary origin for kangite (Ma et al., 2013). The Fe-enrichment of spinel that coexists with kangite does support this interpretation (Ma et al., 2013). In SaU 290, however, cryptocrystalline chondrules are common and almost all glass or mesostasis in chondrules remain intact (Zhang et al., 2007; Zhang and Hsu, 2009). And no spinel and forsterite grains contain Fe-rich rims (Zhang and Hsu, 2009). No evidence involving oxidation was observed in SaU 290 (Zhang and Hsu, 2009). Lack of oxidation in SaU 290 argues against that the low Ti³⁺/Ti^{tot} values in panguite and anosovite in A0031 are a product of oxidation. If panguite and anosovite in A0031 originally had a Ti³⁺/Ti^{tot} value similar to that of Ti-rich davisite, their oxidation must at least have resulted in a change of volume and fractures would form during this process because that Ti is a dominant element in both panguite and anosovite. However, no such evidence is present in A0031. Therefore, a secondary origin (scenario 1) for the various Ti³⁺/Ti^{tot} values in different Ti-rich minerals seems unlikely.

Ma et al. (2012) suggested that the various Ti³⁺/Ti^{tot} values for panguite and surrounding Ti-rich davisite in Allende are primary features. However, they considered that panguite and surrounding Ti-rich davisite might not be genetically related. If this is the case, panguite, anosovite, and Ti-rich davisite in A0031 may not be genetically related as well. The various Ti³⁺/Ti^{tot} values might reflect a large change of redox conditions during condensation of CAI minerals from the nebula. However, the petrographic observations argue against this interpretation. First, hexaferrum grains occur as inclusions in all these three minerals (Fig. 1). This texture indicates that these three minerals condensed at a common location and probably nucleated on hexaferrum grains. Second, similar enrichment of Ti, Sc, and Al in these three minerals supports that they have formed in a common Ti-, Sc-, Al-rich system. If panguite, anosovite, and Ti-rich davisite formed under different redox conditions, the chemical conditions from which these minerals formed might also be different and enrichment of Ti, Sc, and Al in all these three minerals would not be observed. Therefore, the scenario 2 seems also unlikely for the case of A0031. Thus, we consider that the scenario 3 might be the most likely.

However, only difference in ionic radii cannot account for the observed distribution of Ti^{3+} and Ti^{4+} among panguite, anosovite, and Ti-rich davisite. Ma et al. (2012) have discussed the possible effects of ionic radii. They found that the ionic radius of Ti^{3+} for octahedral site is smaller than that of Y^{3+} and larger than that of Al^{3+} ; both Y^{3+} and Al^{3+} are present with high concentrations in panguite (Ma et al., 2012). So, Ti^{3+} should be able to incorporate into the crystal structure of panguite, if only based on its ionic radius. Ti_3O_5 is also a stable phase that has been synthesized in laboratory (e.g., Onoda, 1998) and observed in a chondrite (Brearley, 1993). Ti^{3+} is also present in the anosovite phase from A0031, although the $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ value in anosovite is less than that in Ti-rich davisite. These facts imply that ionic radii are not the dominant and only factor controlling the distribution of Ti^{3+} and Ti^{4+} among panguite, anosovite, and Ti-rich davisite, at least for the latter two phases. Given that panguite, anosovite, and Ti-rich davisite in A0031 and the counterpart in Allende 12A (Ma et al., 2012) are complex solid solutions, we suspect that the various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values are related to various competition abilities of Sc, Al, and Ti^{3+} to incorporate into in different minerals when these phases condensed from the solar nebula. Laboratory simulation experiments are needed to test this possibility.

Although the Ti-rich minerals in A0031 have various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values, the presence of Ti^{3+} in anosovite and Ti-rich davisite indicates that this CAI formed in a highly reducing nebular setting. If we compare the average $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ value for Ti-rich davisite with those in other refractory inclusions from carbonaceous chondrites (e.g., Simon and Grossman, 2006, 2011; Simon et al., 2007, 2008, 2012; Ma and Grossman, 2009a, 2009b; Ma et al., 2012, 2013; Zhang and Yurimoto, 2013), most Ti-rich pyroxene grains ($\text{TiO}_2 > 4$ wt%) have a peak at ~ 0.6 for $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ value. This similarity indicates that the redox conditions of the nebular setting where refractory inclusions from different carbonaceous chondrites formed could be very similar although subtle variations cannot be excluded.

5. CONCLUSIONS

1. We performed a detailed mineralogical analysis and a SCAPS oxygen isotope

mapping on a Ti-Sc-rich refractory inclusion A0031 from the CH chondrite SaU 290. Based on the petrographic texture and comparison with theoretical results, we consider that A0031 has a condensation origin and its formation can be divided into four stages. The first stage includes the condensation of hexaferrum, perovskite, and spinel. The second stage includes the formation of panguite, anosovite, Ti-rich davisite, and anorthite. The third stage is the formation of Al-Ti-rich diopside and the forth stage is the formation of enstatite.

2. Panguite in A0031 is its third occurrence in nature. Anosovite is the second occurrence of Ti_3O_5 in nature, as a new **ultrarefractory** mineral formed in the solar nebula. Its presence in a CAI confirms the stability of this phase in the early solar nebular setting and supports the expectation of equilibrium condensation models.
3. Based on the pristine nature of A0031, we exclude the secondary origin of panguite and Ti-Sc-rich pseudobrookite-structure phase. We suggest that the various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values of panguite, anosovite, and Ti-rich davisite are primary features of A0031. The texture and compositional feature of panguite, anosovite, and Ti-rich davisite indicate that they have formed in a common nebular location, arguing against that they formed in different nebular location and then mixed with each other. We propose that the various $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values for different minerals could be controlled by various competition abilities of Sc, Al, and Ti^{3+} to incorporate into panguite, anosovite, and davisite.
4. The Ti-rich davisite in A0031 has $\text{Ti}^{3+}/\text{Ti}^{\text{tot}}$ values similar to those of other Ti-rich Ca-clinopyroxenes in refractory inclusions, indicating the redox conditions of solar nebular settings where these Ti-rich Ca-pyroxenes formed are similar.

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Figure 1. Back-scattered electron image of the Ca,Al-rich inclusion (A0031) containing anosovite, panguite, hexaferrum, davisite, Ti,Al-rich diopside, anorthite, spinel, perovskite, and enstatite.

Figure 2. Enlarged BSE image showing anosovite with panguite included in davisite.

Figure 3. BSE image (A) of A0031 and X-ray maps of Ca (B), Ti (C), and Al (D).

Figure 4. EBSD pattern of the labelled panguite crystal and the pattern indexed with the orthorhombic $Pbca$ structure.

Figure 5. EBSD pattern of the labelled anosovite crystal in Figure 2 and the pattern indexed with the $Bbmm$ Sc_2TiO_5 structure.

Figure 6. BSE image (A) of a typical region in A0031 and X-ray maps of Ti (B), Y (C), and Zr (D).

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Figure. 7. BSE image (a) and $\delta^{18}\text{O}$ isotopograph (b) of A0031. The high- $\delta^{18}\text{O}$ rim could be caused by large variation of O concentration at the margin of A0031 during sputtering. The unit of $\delta^{18}\text{O}$ in the color bar is permil.

745 Table 1. EPMA compositions of Ti-rich davisite and Al,Ti-rich diopside in A0031

wt%	Ti-rich davisite					Al,Ti-rich diopside			
	19	20	21	22	23	24	25	26	27
Sc ₂ O ₃	8.40	8.32	8.64	10.32	10.03	2.96	2.65	3.28	4.12
ZrO ₂	1.15	1.23	1.13	1.89	1.53	0.43	0.24	0.59	0.49
CaO	22.88	22.87	22.77	22.96	21.88	21.64	21.00	22.22	22.76
TiO ₂	4.07	4.63	3.57	2.64	3.59	2.31	1.95	2.93	3.48
Ti ₂ O ₃ *	5.09	4.52	5.02	5.47	7.85	0.00	0.00	0.00	0.00
Al ₂ O ₃	18.08	18.09	18.39	19.39	18.86	4.33	3.85	5.53	7.07
FeO	1.20	1.28	0.72	0.64	0.66	1.25	1.33	0.76	0.63
V ₂ O ₃	0.83	0.80	0.94	1.03	1.08	0.30	0.26	0.27	0.45
Cr ₂ O ₃	0.45	0.40	0.54	0.35	0.54	0.48	0.55	0.52	0.43
MgO	5.95	6.01	5.94	4.66	4.86	15.45	16.39	14.82	13.86
SiO ₂	30.83	30.52	30.68	29.30	27.88	49.32	50.15	48.57	46.52
Y ₂ O ₃	0.91	0.61	0.60	1.02	1.02	0.55	0.04	0.26	0.29
Totals	99.84	99.29	98.94	99.67	99.78	99.03	98.41	99.77	100.09
Based on 6 O atoms									
Sc	0.284	0.282	0.293	0.352	0.343	0.095	0.085	0.105	0.132
Zr	0.019	0.021	0.019	0.032	0.026	0.007	0.004	0.009	0.008
Ca	0.951	0.954	0.951	0.963	0.921	0.855	0.829	0.872	0.895
Ti ⁴⁺	0.119	0.136	0.105	0.078	0.106	0.064	0.054	0.081	0.096
Ti ³⁺	0.165	0.147	0.164	0.179	0.257	0.000	0.000	0.000	0.000
Al	0.826	0.830	0.845	0.894	0.873	0.188	0.167	0.239	0.306
Fe	0.039	0.042	0.023	0.021	0.022	0.038	0.041	0.023	0.019
V	0.026	0.025	0.029	0.032	0.034	0.009	0.008	0.008	0.013
Cr	0.014	0.012	0.017	0.011	0.017	0.014	0.016	0.015	0.013
Mg	0.344	0.349	0.345	0.272	0.285	0.849	0.901	0.809	0.758
Si	1.195	1.189	1.196	1.146	1.095	1.819	1.849	1.779	1.708
Y	0.019	0.013	0.012	0.021	0.021	0.011	0.001	0.005	0.006
Ti ³⁺ /Ti ^{tot}	0.58	0.52	0.61	0.70	0.71	0.00	0.00	0.00	0.00

746 Ti₂O₃*: calculated on the stoichiometry assumption of pyroxene

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Table 2. EPMA compositions of anosovite and panguite in A0031

	Anosovite		Panguite		
	Grain-1	Grain-2	This study	Ma et al. (2012)	
wt%	N=4*	N=6	N=3	N=5	N=4
MgO	6.50 (0.12)†	6.28 (0.14)	4.55 (0.03)	5.54	1.98
Al ₂ O ₃	4.51 (0.08)	5.22 (0.19)	8.76 (0.27)	7.58	5.94
SiO ₂	0.94 (0.13)	0.99 (0.10)	1.34 (0.06)	1.89	5.04
CaO	1.15 (0.12)	1.47 (0.06)	4.19 (0.13)	3.34	8.73
Sc ₂ O ₃	8.38 (0.11)	9.92 (0.16)	14.42 (0.13)	10.67	5.97
TiO ₂	50.99 (0.58)	50.39 (0.67)	48.36 (0.33)	47.97	30.68
Ti ₂ O ₃	21.45 (0.24)	17.87 (0.42)	3.16 (0.37)		
V ₂ O ₃	1.58 (0.10)	1.77 (0.10)	1.46 (0.05)	0.95	0.27
Cr ₂ O ₃	0.93(0.05)	1.08 (0.11)	2.31 (0.05)	0.54	
FeO	1.04 (0.17)	1.02 (0.13)	0.96 (0.16)	1.81	2.21
Y ₂ O ₃	0.16 (0.16)	1.26 (0.26)	4.59 (0.02)	5.38	10.16
ZrO ₂	1.41 (0.15)	2.40 (0.33)	4.51 (0.10)	14.61	25.92
Total	99.04	99.66	100.67	100.28	96.9
	Based on 5 O atoms		Based on 3 O atoms		
Mg ²⁺	0.345	0.333	0.147		
Al ³⁺	0.189	0.219	0.226		
Si ⁴⁺	0.033	0.035	0.029		
Ca ²⁺	0.044	0.056	0.098		
Sc ³⁺	0.260	0.307	0.273		
Ti ⁴⁺	1.365	1.347	0.791		
Ti ³⁺	0.637	0.531	0.057		
V ³⁺	0.045	0.050	0.026		
Cr ³⁺	0.026	0.030	0.040		
Fe ²⁺	0.031	0.030	0.017		
Y ³⁺	0.003	0.024	0.053		
Zr ⁴⁺	0.022	0.037	0.042		
Ti ³⁺ /Ti ^{tot}	0.32	0.28	0.07		

*Number of analyses.

†Numbers in parentheses represent one standard deviation of the mean for the n analyses conducted on the phase.

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Table 3. Calculated X-ray powder diffraction data ($I_{\text{rel}} > 5\%$) for the anosovite in SaU 290.

h	k	l	$d [\text{\AA}]$	I_{rel}
1	1	0	3.544	100
0	2	2	3.506	7
1	1	1	3.340	37
1	1	2	2.890	14
0	2	3	2.758	24
0	0	4	2.497	17
1	3	0	2.483	15
0	2	4	2.227	18
0	4	2	2.208	25
1	1	4	2.041	6
0	4	3	1.979	20
2	0	0	1.899	37
1	3	4	1.761	42
1	5	2	1.650	22
2	2	3	1.564	7
1	3	5	1.557	6
1	5	3	1.548	9
2	0	4	1.512	7
2	2	4	1.445	7
2	4	2	1.440	11
0	2	7	1.370	6
2	4	3	1.370	9
1	1	7	1.324	7
1	7	2	1.275	11
2	2	7	1.111	6
3	3	4	1.068	7
1	9	5	0.930	6
3	7	2	0.925	5