

Definition and range of composition of naturally occurring minerals with the pseudobrookite structure

JOHN F. W. BOWLES

Department of Earth Sciences, Open University, Walton Hall, Milton Keynes, Buckinghamshire MK7 6AA, England

ABSTRACT

Pseudobrookite, armalcolite, Ti_3O_5 , and “kennedyite” all have the pseudobrookite structure and, besides Ti, Fe, and oxygen, can contain appreciably concentrations of additional elements (Cr, Al, V, Mn, Ca, Zr, etc.). The compositional range of these minerals has never been adequately defined, and there is some confusion in the literature that leaves room for further misunderstanding. A survey of the principal analyses of pseudobrookite, armalcolite, “anosovite” (Ti_3O_5), and “kennedyite” leads, in this paper, to a definition of the range of composition of these minerals, based on established practice and chemically defined boundaries.

“Kennedyite” is an unnecessary name that is now discarded. Pseudobrookite is defined as having an ideal formula of Fe_2TiO_5 with a composition limited by $FeTi_2O_5$, $FeMg_{0.5}Ti_{1.5}O_5$, and intermediate compositions. Armalcolite has an ideal formula $Fe_{0.5}Mg_{0.5}Ti_2O_5$ with a compositional range limited by $MgTi_2O_5$, $FeTi_2O_5$, $FeMg_{0.5}Ti_{1.5}O_5$, and $Mg_{0.5}Ti_{2.5}O_5$ and including intermediate compositions.

These proposals have been submitted to the IMA Commission on New Minerals and Mineral Names, and the commission has given its approval.

INTRODUCTION

Pseudobrookite (Fe_2TiO_5) is well established as a naturally occurring mineral (Koch, 1878; Groth, 1879; Dana, 1892). It has an orthorhombic structure that was first described by Pauling (1930). Akimoto et al. (1957) and Haggerty and Lindsley (1970) have investigated the solid-solution series between pseudobrookite and $FeTi_2O_5$. A number of other phases have been shown to have the same structure including tielite (Al_2TiO_5 ; Yamaguchi, 1944) and synthetic phases such as Sc_2TiO_5 (Ito, 1971) and Fe_2ZrO_5 (Supe and Rao, 1974). $MgTi_2O_5$ has a pseudobrookite structure, and the solid solution between $MgTi_2O_5$ and $FeTi_2O_5$ was studied by Moore and Sigurdson (1949) and Lindsley et al. (1974). Solid solution between Al_2TiO_5 and $MgTi_2O_5$ was examined by Sigurdson and Cole (1949). Attempts have been made to provide mineral names for $MgTi_2O_5$ (“karrooite”; von Knorring and Cox, 1961; or “Mg-pseudobrookite”) and $FeTi_2O_5$ (“ferropseudobrookite”; Agrell and Long, 1960), but these names have no standing in mineralogy (Fleischer, 1970). “Anosovite” (Ti_3O_5) has the pseudobrookite structure and has been synthesized and described from slags (Belyankin and Lapin, 1951; Rusakov and Zhdanov, 1951; Zhdanov and Rusakov, 1952). The solid solution from Ti_3O_5 to $FeTi_2O_5$ has been studied by Grey and Ward (1973) and Navrotsky (1975).

Naturally occurring minerals with the pseudobrookite structure have intermediate compositions so that in addition to varying proportions of Fe^{2+} and Fe^{3+} (Ottmann and Frenzel, 1965), Mg, Mn, Al, and Cr frequently

occur. “Kennedyite” ($Fe_2MgTi_3O_{10}$) was described by von Knorring and Cox (1961) from a locality in the Karroo sills of the Mateke Hills, Zimbabwe, where it forms a significant proportion of the rock. Haggerty (1976) examined samples from the same locality and commented on the similarity of the oxide assemblage and mineral compositions to that of armalcolite-bearing high-Ti basalts.

The first Apollo landing provided the mineral armalcolite ($Fe,MgTi_2O_5$) from Mare Tranquillitatis (Anderson et al., 1970). It has been recognized that both tan and gray armalcolite occur since different properties have been described in reflected light (Haggerty, 1973a), but no chemical or structural distinction can be made between them (Smyth, 1974; Williams and Taylor, 1974; El Goresy et al., 1974) so the terms “ortho-armalcolite” and “para-armalcolite” (Haggerty, 1973a) are not recognized (Fleischer, 1974). Cr- and Zr-bearing phases occur that appear to be either Cr- and Zr-rich armalcolite or a Cr- and Zr-bearing phase similar to armalcolite but as yet unnamed (Steele and Smith, 1972; Levy et al., 1972; Wechsler et al., 1976; Haggerty, 1983). Armalcolite also occurs elsewhere on the Moon, on Earth, and in meteorites, where it is formed under reducing conditions. Natural armalcolite can contain a proportion of either Ti^{3+} or Fe^{3+} .

Figure 1 represents the recognized iron-titanium-magnesium oxides with the pseudobrookite structure and illustrates the problems brought about by the manner in which the subject has developed. These are that central components rather than end members have been named,

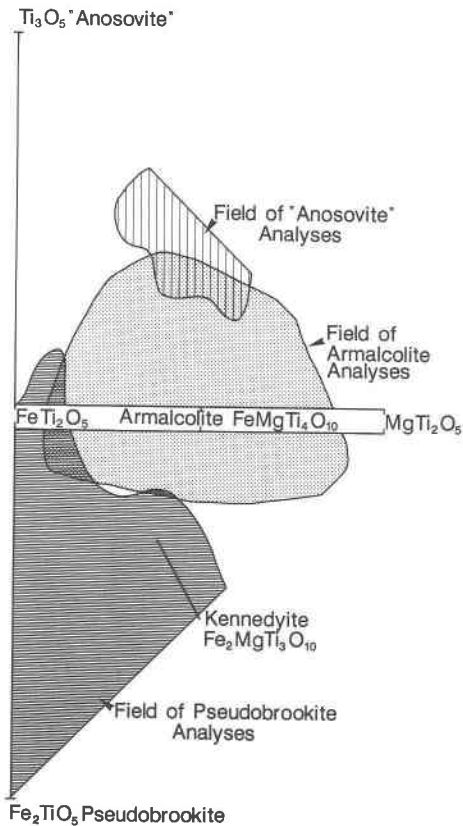


Fig. 1. Previously recognized iron-titanium-magnesium oxide minerals with pseudobrookite structure.

and there is no clear boundary between the various named phases.

Natural pseudobrookites showing all compositions between Fe_2TiO_5 and FeTi_2O_5 occur (Ottemann and Frenzel, 1965), and some contain appreciable Mg. It has not been clear how close natural pseudobrookites approach "kennedyite" or where a distinction should be drawn. Some phases, described as pseudobrookite are more Mg-rich than "kennedyite." The situation concerning armalcolite shows similar uncertainty. When armalcolite was defined (Anderson et al., 1970), the presence of Ti^{3+} in solid solution was not appreciated. The apparent nonstoichiometry was attributed to a cation deficiency. The Fe^{3+} content of armalcolite was discussed by Anderson et al. (1970), and they contended that "a low content of Fe_2O_3 in armalcolite is obviously essential for its recognition as a new mineral" while recognizing that the rocks in which the lunar type material crystallized were formed under highly reducing conditions and that Fe^{3+} is absent in those rocks. It was soon appreciated (Lindsley et al., 1974; Kesson and Lindsley, 1975) that a significant Ti^{3+} component is frequently present in armalcolite and found to provide a better explanation of the properties than cation deficiency. Once this step had been taken, there seems to have been an assumption by some authors that the definition of armalcolite excludes Fe^{3+} although, as will be

shown later, the analyses of the type material (Anderson et al., 1970) show a range of compositions including both Ti^{3+} - and Fe^{3+} -bearing members. Thus a description by Velde (1975) of an armalcolite containing Fe^{3+} was criticized by El Goresy and Chao (1976) with the statement that this "ferri-armalcolite . . . contains 7.45% Fe_2O_3 " and that "therefore it is not an armalcolite but a member of the pseudobrookite series." Some of the analyses given by El Goresy and Chao (1976) and described as armalcolite contain almost as much Fe^{3+} as the mineral described by Velde (1975) so this statement is inconsistent, but it illustrates the combined problems of determining $\text{Fe}^{2+}/\text{Fe}^{3+}$ from electron-microprobe analyses, which only give total Fe, and the lack of definition of the armalcolite boundary.

The analyses reported for "anosovite" (Belyankin and Lapin, 1951; Lapin et al., 1956; Rudneva and Malysheva, 1957) have a high Al content (4–12% Al_2O_3) and contain comparatively little Fe (1–9% FeO). They are principally composed of Ti_3O_5 and $(\text{Mg}, \text{Mn}, \text{Ca})\text{Ti}_2\text{O}_5$ with minor FeTi_2O_5 , but appreciable $(\text{Al}, \text{Cr}, \text{V})_2\text{TiO}_5$. There is, therefore, a compositional similarity between these "anosovites" and the Cr-Zr-Ca-bearing armalcolites distinguished only by a lack of Zr, higher Ti^{3+} , and lower Fe^{2+} in the "anosovites."

PSEUDOBROOKITE- FeTi_2O_5 - Ti_3O_5

Studies of the geometry of the Fe-Ti-O system (Thompson, 1982; Gorter, 1957; Lindsley, 1976) have shown that reduced phases such as Ti_2O_3 and Ti_3O_5 can be included on a diagram with FeO, TiO_2 , and Fe_2O_3 . In these constructions, the solid-solution series between pseudobrookite and FeTi_2O_5 (Akimoto et al., 1957) and the Ti_3O_5 to FeTi_2O_5 solid-solution series (Grey and Ward, 1973) appear as a single contiguous series. The implication is that it is possible to describe pseudobrookite, FeTi_2O_5 , and Ti_3O_5 as a single series from pseudobrookite to Ti_3O_5 . Structurally, the solid-solution series from pseudobrookite to FeTi_2O_5 and from FeTi_2O_5 to Ti_3O_5 are well established so there is no practical difficulty in considering one as a continuation of the other. The series from pseudobrookite to Ti_3O_5 represents a steady replacement of Fe by Ti with reduction first of Fe^{3+} to Fe^{2+} and then of some of the Ti^{4+} to Ti^{3+} . This view of the replacement process is supported by studies of the site occupancy within the structure (Grey and Ward, 1973; Virgo and Huggins, 1975; Navrotsky, 1975). The structure is disordered and the degree of disorder is temperature dependent, (Wechsler, 1977) but the results (Table 1) indicate progressive substitution of Fe^{3+} by Fe^{2+} leading to complete removal of Fe^{3+} followed by substitution of Ti^{4+} by Ti^{3+} .

The idea that pseudobrookite to Ti_3O_5 is a single series has been implicit in the work of the authors already mentioned or has been more or less explicitly stated in their work. It needs to be restated here in discussion of the nomenclature. The benefit is that FeTi_2O_5 becomes an intermediate composition rather than an end member,

TABLE 1. Site occupancy of pseudobrookite, FeTi_2O_5 , and Ti_3O_5

	M1 (4c)				M2 (8f)				Reference
	Fe^{3+}	Fe^{2+}	Ti^{4+}	Ti^{3+}	Fe^{3+}	Fe^{2+}	Ti^{4+}	Ti^{3+}	
Pseudobrookite	3.52	—	0.48	—	4.48	—	3.52	—	Virgo and Huggins (1975)
FeTi_2O_5	—	2.72	1.28	—	—	1.28	6.72	—	Virgo and Huggins (1975)
FeTi_2O_5	—	2.88	1.12	—	—	1.12	6.88	—	Grey and Ward (1973)
FeTi_2O_5	—	3.24	0.76	—	—	0.76	7.24	—	Navrotsky (1975)
Ti_3O_5	—	—	0.20	3.80	—	—	3.80	4.20	Navrotsky (1975)

and concern as to whether it should have a name diminishes.

There is a need for clearly defined boundaries in the pseudobrookite system, and these should be defined on the basis of simple chemical parameters while offering minimum unnecessary disturbance to the existing literature.

It is clear that there is no structural or chemical reason why the solid-solution series pseudobrookite to FeTi_2O_5 and FeTi_2O_5 to Ti_3O_5 , which have previously been described separately, should not be considered as a single solid-solution series pseudobrookite to Ti_3O_5 . Indeed, the discussion above of the chemistry and structure of the naturally occurring minerals in this group indicates good reasons for such an amalgamation.

The system consists of five components, Fe^{3+} , Fe^{2+} , Mg^{2+} , Ti^{4+} , and Ti^{3+} . Ti^{4+} is common to all the pseudobrookite-type minerals while Fe^{3+} and Ti^{3+} are mutually exclusive. The system can then be reduced to three independent variables. It is, therefore, possible to represent the minerals in terms of two-dimensional space by using a straight line to represent the series pseudobrookite- FeTi_2O_5 - Ti_3O_5 and using the second dimension to indicate the MgTi_2O_5 contents. Thus the pseudobrookite- Ti_3O_5 series can be represented by the hypotenuse of a right-angled triangle with MgTi_2O_5 at the right angle and FeTi_2O_5 in the center of the hypotenuse. Lines from $\text{FeMg}_{0.5}\text{Ti}_{1.5}\text{O}_5$ to FeTi_2O_5 and from $\text{Mg}_{0.5}\text{Ti}_{2.5}\text{O}_5$ to FeTi_2O_5 represent equal proportions of the two adjacent end-member compositions and varying proportions of FeTi_2O_5 . Because the Fe^{3+} and the Ti^{3+} are mutually exclusive, the location of compositions within the two halves of this triangle must be calculated independently. The first step of such a calculation is, therefore, to determine which half (Fe^{3+} - or Ti^{3+} -bearing) of the triangle contains the mineral analysis. Details of this calculation are given in Appendix 1.

RANGE OF COMPOSITION

Previously, the names pseudobrookite, armalcolite, "kennedyite," and "anosovite" have referred to specific compositions with no defined range of variation although solid-solution series were known to exist between these phases to the extent that has already been described. There has been some confusion in the literature concerning the nomenclature of intermediate phases. Any attempt to introduce a definition at this stage must be arbitrary but should also be based on common usage. Analyses of ar-

malcolite, pseudobrookite, "anosovite," and "kennedyite" from the literature have been plotted in Figure 2 after recalculation of their end-member compositions (see App. 1) to ensure that they have all been treated alike. Figure 2 places the pseudobrookite- Ti_3O_5 series at the left-hand side with FeTi_2O_5 placed centrally. The series FeTi_2O_5 to MgTi_2O_5 is drawn at right angles to pseudobrookite- Ti_3O_5 . Mn and Ca have been plotted with Mg. Each phase is plotted in this two-dimensional field without taking into account any $(\text{Al,Cr,V})_2(\text{Ti,Zr})\text{O}_5$ component. Where no Al, Cr, or V are reported in the analysis, the phase is represented as a point. In order to illustrate the Al, Cr, V, and Zr contents when they are reported, a diagonal line has been used that is proportional in length to the $(\text{Al,Cr,V})_2(\text{Ti,Zr})\text{O}_5$ content. The lower end of the line represents the analysis excluding Al, Cr, V, and Zr. The observer may view these lines as standing in the third dimension.

CONCLUSIONS

The results of the following conclusions are shown in Figure 2 with analyses of relevant phases from the literature.

"**Kennedyite.**" This mineral name has been little used and only in reference to one geographical location. There is significant disparity between the composition of the type material and the ideal formula. Phases of this composition show great similarity with armalcolite (Haggerty, 1976). "Kennedyite" is an unnecessary name for a mineral of the pseudobrookite solid-solution series and a composition intermediate between Fe_2TiO_5 , MgTi_2O_5 , and FeTi_2O_5 . The name should be discarded, and the composition of the type material included within the armalcolite field.

The armalcolite-pseudobrookite boundary. This should be drawn from $\text{FeMg}_{0.5}\text{Ti}_{1.5}\text{O}_5$ to FeTi_2O_5 to represent equal proportions of MgTi_2O_5 and Fe_2TiO_5 for varying FeTi_2O_5 contents. Most of the current usage is unchanged by this boundary. Notable exceptions are (1) "kennedyite" (von Knorring and Cox, 1961) becomes armalcolite; (2) analyses of pseudobrookite nos. 27, 28, and 29 (29 from "kennedyite" type locality; Ottemann and Frenzel, 1965) become armalcolite; and (3) analysis of pseudobrookite no. 9 (Frenzel, 1971), which contains significant Ti^{3+} , becomes armalcolite. The Fe^{3+} -rich armalcolites of El Goresy and Chao (1976), Velde (1975), Pedersen (1979), and Tarasov et al. (1973) remain as armalcolite.

The armalcolite- Ti_3O_5 boundary. This should be drawn

Fig. 2. Definition of mineral compositions for iron-titanium-magnesium oxide minerals with pseudobrookite structure. The left-hand axis shows pseudobrookite to "anosovite" as a single series and minerals containing Mg, Mn, and Ca as a $(\text{Mg,Mn,Ca})\text{Ti}_2\text{O}_5$ molecule are plotted to the right. Those minerals plotted above the FeTi_2O_5 to $(\text{Mg,Mn,Ca})\text{Ti}_2\text{O}_5$ join contain Ti^{3+} , whereas those below that join contain Fe^{3+} . The calculation of composition is detailed in App. 1. Minerals containing some of the $(\text{Al,Cr,V})_2(\text{Ti,Zr})\text{O}_5$ molecule are represented by a line that is proportional in length to the amount of that molecule present. The lower end of the line represents the location of the mineral in Fe-Ti-(Mg,Mn,Ca) oxide space. The lines are true length, not projections, but give a three-dimensional impression if viewed at an angle. If the mineral contains no $(\text{Al,Cr,V})_2(\text{Ti,Zr})\text{O}_5$, it is represented by a point. Boundaries have been added as described in the text. Within the armalcolite field, further informal divisions have been added; these are lunar Cr-Zr-Ca armalcolite and lunar Zr-armalcolite following Haggerty (1973b) whereas remaining armalcolite is here divided into lunar armalcolite and terrestrial and meteoritic armalcolite. The sources of the data are detailed below, and analyses renamed here or close to mineral boundaries are indicated by numbering in the diagram.

Pseudobrookite field. Ottemann and Frenzel (1965): analyses 1–26 (nos. 15, 22, and 23 in Fig. 2). Frenzel (1971): analyses 1, 5, and 8 (repeat of above analyses 24, 25, and 26). Lufkin (1976): mean of five similar analyses. Smith (1965): samples 92420, 92424, 92425, 92427, 92431.

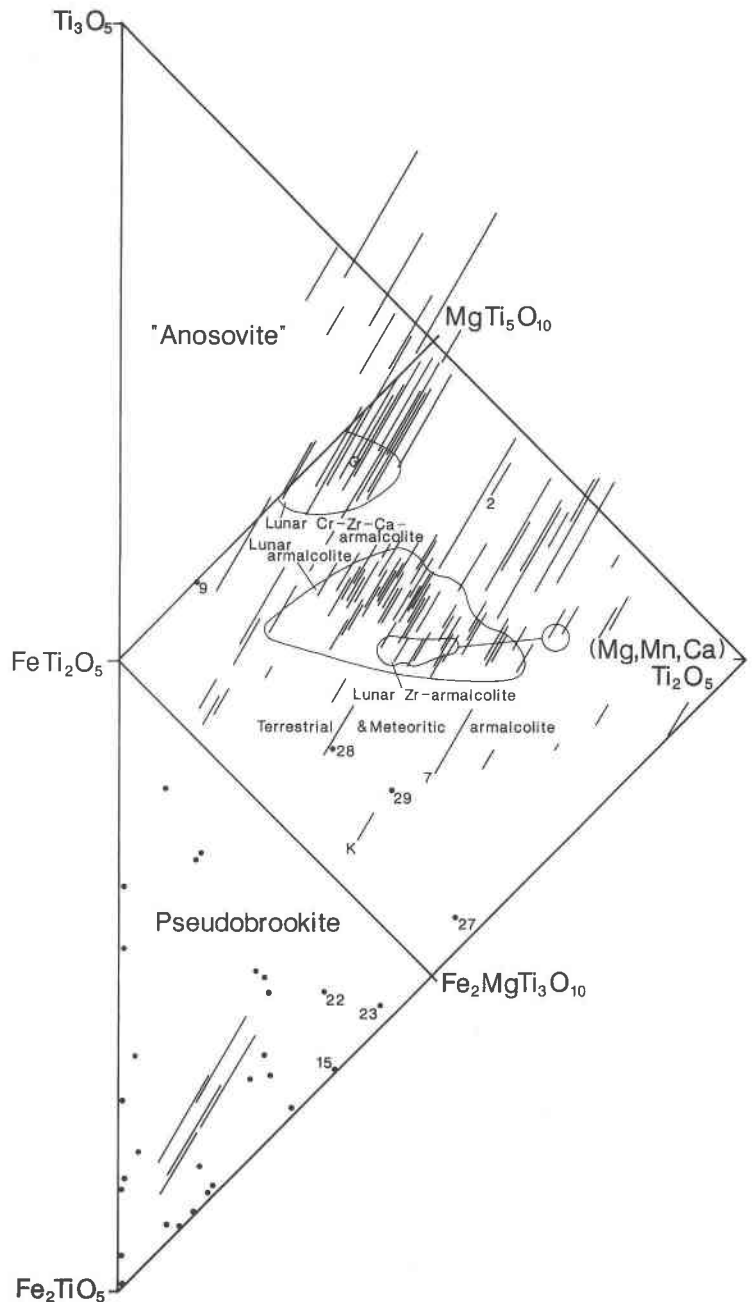
Armalcolite field—Lunar Cr-Zr-Ca armalcolite. Brown et al. (1972) described as "mineral X." Brown et al. (1973): mean of four similar analyses. Haggerty (1973b): analyses 1, 2, 3, 8, 9. Steele and Smith (1972): analyses 5–7. Steele (1974): analyses 25a, 25b, 25c. Levy et al. (1972): "pseudoarmalcolite"—considered by the authors to be a different phase. Lapin et al. (1956): sample 3349 originally described as anosovite, indicated by 3 in Fig. 2.

Armalcolite field—Lunar armalcolite. Anderson et al. (1970): analyses 1a₁, 1a₂, 1b₁, 1b₂, 2, 3a, 3b, 4, 5, 6. Akimoto et al. (1970): 1150 and 1175 °C experimental melting of lunar rock. Agrell et al. (1970): no analysis number. Haggerty (1973a): "ortho-" and "para-" armalcolite. Haggerty (1973b): analyses 1, 2, 3, 4. Tarasov et al. (1973): analyses 876-4, 876-5. El Goresy et al. (1974): analyses 1–8. Papike et al. (1974): analyses 1–7. Smyth (1974): O and P. Williams and Taylor (1974): O and P. Wechsler et al. (1976) and Stanin and Taylor (1980): analyses A, B, C, D.

Armalcolite field—Zr-armalcolite. Steele (1974): analyses 3, 7, 11a, 11b, 12, 16a, 16b. Haggerty (1973b): analyses 1, 2, 3, 4.

Armalcolite field—Terrestrial and meteoritic armalcolite. von Knorring and Cox (1961): specimen F7168/C888, originally "kennedyite" (indicated by K in Fig. 2). El Goresy and Chao (1976): analyses 1, 3, 5, 7, 8, 9. Velde (1975) and Haggerty (1975): no analyses numbers. Haggerty (1978): 1, 3, high-Ca unknown mineral 10. Haggerty (1983): 104-6, 104-7, 113-10. Tsymbal et al. (1980): 1–3. Pedersen (1979): 1–8. Akimoto et al. (1970): synthesized from lunar rock at 1200 °C and 1 atm. Ottemann and Frenzel (1965): analyses 27–29 (originally pseudobrookite; shown by corresponding numbers in Fig. 2). Smith (1965): sample 75385 (originally pseudobrookite; shown as 7 in Fig. 2; see App. Table 1). Frenzel (1971): analysis 9 (originally pseudobrookite; shown as 9 in Fig. 2). Belyankin and Lapin (1951): sample 2289 originally "anosovite" (shown as 2 in Fig. 2). Haggerty (1978): high-Ca unknown mineral 1.

Ti₃O₅ ("anosovite") field. Lapin et al. (1956): samples 3319, 3341, 3353. Belyankin and Lapin (1951): sample 2406. Rudneva and Malysheva (1957): samples 170, 172, 228.



from $Mg_{0.5}Ti_{2.5}O_5$ to $FeTi_2O_5$ and represents equal proportions of $MgTi_2O_5$ and Ti_3O_5 . The majority of the mineral descriptions in the literature are unchanged by the choice of this boundary except the analyses of "anosovite" no. 2289 (Belyankin and Lapin, 1951) and "anosovite" no. 3349 (Lapin et al. 1956) plot well within the armalcolite field and should be known as armalcolite.

Definition of pseudobrookite. The boundaries defined above permit pseudobrookite to be defined to have the ideal end-member formula Fe_2TiO_5 and a compositional range limited by $FeTi_2O_5$, $FeMg_{0.5}Ti_{1.5}O_5$, and compositions between these limits. Pseudobrookite is orthorhombic and in space group *Bbmn*. It has unit-cell parameters approximating $a = 9.767$, $b = 9.947$, and $c = 3.717$ Å.

Definition of armalcolite. Similarly, armalcolite can now be defined to have the ideal formula $Fe_{0.5}Mg_{0.5}Ti_2O_5$ and a compositional range limited by $MgTi_2O_5$, $FeMg_{0.5}Ti_{1.5}O_5$, $FeTi_2O_5$, $Mg_{0.5}Ti_{2.5}O_5$, and compositions between these limits. Armalcolite is orthorhombic and in space group *Bbmn*. It has unit-cell parameters approximating $a = 9.743$, $b = 10.024$, and $c = 3.738$ Å.

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APPENDIX 1. METHOD OF CALCULATION OF MINERAL COMPOSITION FROM MICROPROBE ANALYSES

This description and the accompanying example take a microprobe analysis as the starting point. Thus, only total Fe and total Ti are known; the Fe^{3+}/Fe^{2+} and Ti^{4+}/Ti^{3+} ratios are unknown. The first stage of the calculation shows how these ratios may be determined by assuming the mineral to be a stoichiometric mineral in the pseudobrookite plane. This initial procedure allows a better total to be obtained, so that one aspect of the quality of the analysis may be judged. The proportion of the appropriate molecules can then be calculated so that the analysis may be plotted in Figure 2.

All elements are expressed as molecular proportions of their standard oxides. MgO , MnO , and CaO are combined to form MO , and Al_2O_3 , Cr_2O_3 , and V_2O_5 are put together to form R_2O_3 . Determine x , where $x = (MO + R_2O_3 + FeO)/(TiO_2 + MO + R_2O_3 + FeO)$; if $0 < x < 0.33$, then the phase plots in the upper half of the triangle. For $0.33 < x < 0.67$, the phase plots in the lower half of the triangle. TiO_2 is used to form $MO \cdot 2TiO_2$ and $R_2O_3 \cdot TiO_2$. If $0 < x < 0.33$, the Fe is taken as Fe^{2+} , and formation of $FeO \cdot 2TiO_2$ leaves TiO_2 in excess, which is recalculated as Ti_2O_3 (i.e., $Ti_2O_3 \cdot TiO_2$). If $0.33 < x < 0.67$, then the Ti is left to form TiO_2 , and the Fe is distributed between Fe^{2+} and Fe^{3+} to obtain stoichiometric $FeO \cdot 2TiO_2$ and $Fe_2O_3 \cdot TiO_2$. This procedure is similar to that used by Pedersen (1979) and Kesson and Lindsley (1975) and is satisfactory for most analyses. The Fe^{3+}/Fe^{2+} or Ti^{4+}/Ti^{3+} distribution determined in this way can be calculated back to the initial analysis to find the wt% FeO and Fe_2O_3 (or TiO_2 and Ti_2O_3). The total can then be modified and compared with 100% at this stage to check the quality of the analysis. Occasionally there is insufficient TiO_2 even when all the Fe is taken as Fe^{3+} . In such cases, MnO can be taken as MnO_2 and added to TiO_2 , which helps but is not always completely sufficient to overcome the Ti deficiency in some analyses. It is noticed here that these results lie along the Fe_2TiO_3 - Mg - Ti_2O_3 join. The analyses where ZrO_2 is large are also those where Ti_2O_3 is greatest. It is assumed here that $Ti_2O_3 \cdot ZrO_2$ is formed in these cases. This calculation is illustrated in Appendix Table 1, which takes an analysis from the literature with no preconceived idea as to the Fe^{3+}/Fe^{2+} and Ti^{4+}/Ti^{3+} distribution. The same calculation is repeated in Appendix Table 2 to illustrate the procedure when the Fe^{3+}/Fe^{2+} and Ti^{4+}/Ti^{3+} ratios have been given by the analytical technique.

Plotting the results in Figure 2

The components $FeO \cdot 2TiO_2$, $(Mg, Ca, Mn)O \cdot 2TiO_2$, and $Fe_2O_3 \cdot TiO_2$ or $Ti_2O_3 \cdot TiO_2$ are plotted in the triangle of Figure 2. Readers are familiar with plotting three variables on an equilateral triangle. The principle is the same for the right-angled triangle of Figure 2, and points can be plotted using ordinary squared graph paper. The $MO \cdot 2TiO_2$ percentage is the percentage of the distance from $FeTi_2O_5$ to $(Mg, Mn, Ca)Ti_2O_5$ along that axis, and the Fe_2TiO_3 percentage is the percentage of the distance from $FeTi_2O_5$ to Fe_2TiO_5 . These two distances define a unique point in the lower half of the diagram; the same relation holds for the Ti_2O_3 percentage in the upper half of the diagram. The third quantity, the $FeTi_2O_5$ percentage, could be plotted using contours parallel to the $(Mg, Mn, Ca)Ti_2O_5$ to Fe_2TiO_5 join but in the absence of suitable paper, this confirmation of the position of the point can be omitted. The diagonal line to represent the $(Al, Cr, V)_2(Ti, Zr)O_3$ proportion is drawn on Figure 2 with a length determined by the appropriate percentage (10.96% in example 1) and using the same scale as for the other values plotted. This aspect of the diagram is considered to be illustrative rather than quantitative.

APPENDIX TABLE 1. Example 1

	Wt%	Molecular proportion	R ₂ O ₃ ·TiO ₂	MO·2TiO ₂	Ti left	FeO·2TiO ₂	Fe ₂ O ₃ ·TiO ₂		Corrected analysis (wt%)
TiO ₂	64.13	0.803	0.051	0.412	0.340	0.266	0.074	TiO ₂	64.13
Al ₂ O ₃	5.18	0.051	0.051	—	—	—	—	Al ₂ O ₃	5.18
MgO	8.31	0.206	—	0.206	—	—	—	MgO	8.31
FeO*	20.14	0.280	—	—	—	0.133	—	FeO	9.55
							0.074	Fe ₂ O ₃	11.77
Total	97.76							Total	98.94

	Molecular proportion	4 components (wt%)	3 components (wt%)
FeTi ₂ O ₅	0.133	28.67	32.20
Fe ₂ TiO ₅	0.074	15.90	17.85**
MO·TiO ₂	0.206	44.47	49.94**
R ₂ O ₃ ·TiO ₂	0.051	10.96†	

Note: This analysis is specimen 75385 (Smith, 1965) marked as 7 in Fig. 2. This example is illustrated to three decimal places. It is based on a computer calculation to more decimal places. Some rounding errors will become apparent as the calculation proceeds. Where this occurs, the accurate values have been used. R₂O₃ = Al₂O₃ + Cr₂O₃ + V₂O₅. MO = MgO + MnO + CaO. $x = (MO + R_2O_3 + FeO)/(TiO_2 + MO + R_2O_3 + FeO) = 0.401$. Since $x > 0.33$, keep Ti as Ti⁴⁺ and plot the phase in the lower half of the diagram. (There is not enough TiO₂ to form only FeO·2TiO₂, which would require 0.560TiO₂.) Some Fe must be used up to form Fe₂O₃·TiO₂. Calculate this as follows:

$$\text{molecular proportion of FeO} = 0.280 \text{ (from above)} - 2 \times \text{molecular proportion of Fe}_2\text{O}_3$$

and

$$\text{molecular proportion of TiO}_2 = 2 \times \text{molecular proportion of FeO} + \text{molecular proportion of Fe}_2\text{O}_3.$$

Hence, molecular proportion of TiO₂ = 2(0.280 - 2 × molecular proportion of Fe₂O₃) + molecular proportion of Fe₂O₃ = 0.340 (from above). So molecular proportion of Fe₂O₃ = 0.074 (gives 11.77 wt% Fe₂O₃) and molecular proportion of FeO = 0.266 (gives 9.55 wt% FeO).

* Total Fe expressed as FeO.

** These values are used to determine the point at which the analysis is plotted in Fig. 2.

† Used to determine the length of the diagonal line at same scale.

APPENDIX TABLE 2. Example 2

	Wt%	Molecular proportion	Oxygen proportion	No. of anions	No. of cations	R ₂ O ₃ ·TiO ₂	MO·2TiO ₂	Ti left	FeO·2TiO ₂	Fe ₂ O ₃ ·TiO ₂
TiO ₂	64.13	0.803	1.605	3.463	1.731	0.110	0.890	0.731	0.574	0.159
Al ₂ O ₃	5.18	0.051	0.152	0.329	0.219	0.219	—	—	—	—
MgO	8.31	0.206	0.206	0.445	0.445	—	0.445	—	—	—
FeO	9.55	0.133	0.133	0.287	0.287	—	—	—	0.287	—
Fe ₂ O ₃	11.77	0.074	0.221	0.477	0.318	—	—	—	—	0.318
Total			2.317	5.001						

	Molecular proportion	4 components (wt%)	3 components (wt%)
FeTi ₂ O ₅	0.287	28.67	32.20
Fe ₂ TiO ₅	0.159	15.90	17.85
MO·TiO ₂	0.445	44.47	49.94
R ₂ O ₃ ·TiO ₂	0.110	10.96	

Note: Calculation as example 1 (App. Table 1), but assuming that the Fe³⁺/Fe²⁺ or Ti⁴⁺/Ti³⁺ ratios are known and calculating to 5 oxygen atoms per unit cell.