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

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ABSTRACT

Pseudobrookite, armalcolite, Ti$_2$O$_3$, 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$_3$O$_5$), 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$_2$TiO$_3$, with a composition limited by FeTi$_2$O$_3$, Fe-Mg$_2$Ti$_2$O$_5$, and intermediate compositions. Armalcolite has an ideal formula Fe$_2$Mg$_2$Ti$_2$O$_5$, with a compositional range limited by Mg$_2$Ti$_2$O$_5$, FeTi$_2$O$_3$, FeMg$_2$Ti$_2$O$_5$, and Mg$_2$Ti$_2$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$_2$TiO$_3$) 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$_2$O$_3$. A number of other phases have been shown to have the same structure including tielite (Al$_2$TiO$_4$; Yamaguchi, 1944) and synthetic phases such as Sc$_2$TiO$_3$ (Ito, 1971) and Fe$_2$ZrO$_3$ (Supe and Rao, 1974). Mg$_2$Ti$_2$O$_5$ has a pseudobrookite structure, and the solid solution between Mg$_2$Ti$_2$O$_5$ and FeTi$_2$O$_3$ was studied by Moore and Sigurdson (1949) and Lindsley et al. (1974). Solid solution between Al$_2$TiO$_4$ and Mg$_2$Ti$_2$O$_5$ was examined by Sigurdson and Cole (1949). Attempts have been made to provide mineral names for Mg$_2$Ti$_2$O$_5$ (“karrooite”; von Knorring and Cox, 1961; or “Mg-pseudobrookite”) and FeTi$_2$O$_3$ (“ferropseudobrookite”; Agrell and Long, 1960), but these names have no standing in mineralogy (Fleischer, 1970).

“Aosovite” (Ti$_3$O$_5$) 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$_2$O$_3$ to FeTi$_2$O$_3$ 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$^{3+}$ (Otte-mann and Frenzel, 1965), Mg, Mn, Al, and Cr frequently occur. “Kennedyite” (Fe,MgTi$_2$O$_5$) 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,Mg)Ti$_2$O$_5$ 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,
and there is no clear boundary between the various named phases.

Natural pseudobrookites showing all compositions between Fe$_2$TiO$_4$ and FeTiO$_3$ 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$^{3+}$ 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% FeO,$_{_{7}}$” 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 Fe$^{2+}$/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; Rudnava and Malyshova, 1957) have a high Al content (4–12% Al$_2$O$_3$) and contain comparatively little Fe (1–9% FeO). They are principally composed of Ti$_2$O$_3$ and (Mg, Mn, Ca)Ti$_2$O$_3$ with minor FeTi$_2$O$_5$, but appreciable (Al, Cr, V)Ti$_2$O$_5$. 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$_2$O$_5$-Ti$_2$O$_5$**

Studies of the geometry of the Fe-Ti-O system (Thompson, 1982; Gorter, 1957; Lindsley, 1976) have shown that reduced phases such as Ti$_2$O$_3$ and Ti$_2$O$_5$ can be included on a diagram with FeO, TiO$_2$, and FeO$_3$. In these constructions, the solid-solution series between pseudobrookite and FeTi$_2$O$_5$ (Akimoto et al., 1957) and the Ti$_2$O$_3$ to FeTi$_2$O$_5$, solid-solution series (Grey and Ward, 1973) appear as a single contiguous series. The implication is that it is possible to describe pseudobrookite, FeTi$_2$O$_5$, and Ti$_2$O$_3$ as a single series from pseudobrookite to Ti$_2$O$_3$. Structurally, the solid-solution series from pseudobrookite to FeTi$_2$O$_5$, and from FeTi$_2$O$_5$ to Ti$_2$O$_3$, are well established so there is no practical difficulty in considering one as a continuation of the other. The series from pseudobrookite to Ti$_2$O$_3$ 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$_2$O$_3$, 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$_2$O$_5$, becomes an intermediate composition rather than an end member,
and concern as to whether it should have a name dimin- 
ishes.

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 
in the manner unnecessary disturbance to the existing literature.

It is clear that there is no structural or chemical reason 
why the solid-solution series pseudobrookite to FeTiO₅ 
and FeTiO₅ to TiO₃, which have previously been de- 
scribed separately, should not be considered as a single 
solid-solution series pseudobrookite to TiO₃. 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, Fe³⁺, Fe²⁺, 
Mg²⁺, Ti⁴⁺, and Ti³⁺. Ti⁴⁺ is common to all the pseu-
dobrookite-type minerals while Fe³⁺ and Ti³⁺ are mu-
truly exclusive. The system can then be reduced to three 
independent variables. It is, therefore, possible to repre-
sent the minerals in terms of two-dimensional space by 
using a straight line to represent the series pseudobrook-
ite-FeTiO₅-TiO₃. Mn and Ca have been plotted with Mg. 
Each phase is plotted in this two-dimensional field with-
out taking into account any (Al, Cr, V, Ti, Zr)O₅ compos-

tive. 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 (Al, Cr, V, Ti, Zr)O₅ 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 liter-
are. The 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 com-
position show great similarity with armalcolite (Haggerty, 
1976). “Kennedyite” is an unnecessary name for a min-
eral of the pseudobrookite solid-solution series and a 
composition intermediate between Fe₂TiO₅, Mg₂TiO₅, and 
FeTiO₅. The name should be discarded, and the com-
position of the type material included within the armal-
colite field.

The armalcolite-pseudobrookite boundary. This should 
be drawn from FeMg₂Ti₃O₇ to FeTiO₅ to represent 
equal proportions of MgTiO₅ and Fe₂TiO₅ for varying 
FeTiO₅ contents. Most of the current usage is unchanged 
by this boundary. Notable exceptions are (1) “kennedy-
ite” (von Knorring and Cox, 1961) becomes armalcol-
ite; (2) analyses of pseudobrookite nos. 27, 28, and 29 
(29 from “kennedyite” type locality; Ottmann and Fren-
zel, 1965) become armalcolite; and (3) analysis of pseu-
dobrookite no. 9 (Frenzel, 1971), which contains signif-
icient Ti³⁺ becomes armalcolite. The Fe³⁺-rich armalcolites 
of El Goresy and Cho (1976), Velde (1975), Pedersen 
(1979), and Tarasov et al. (1973) remain as armalcolite.

The armalcolite-TiO₃ boundary. This should be drawn

**Table 1. Site occupancy of pseudobrookite, Fe₂TiO₅, and TiO₃**

<table>
<thead>
<tr>
<th>M1 (4c)</th>
<th>M2 (8f)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pseudobrookite</td>
<td>Fe²⁺</td>
</tr>
<tr>
<td>Fe₂TiO₅</td>
<td>3.52</td>
</tr>
<tr>
<td>FeTiO₅</td>
<td>—</td>
</tr>
<tr>
<td>Fe₂TiO₅</td>
<td>—</td>
</tr>
<tr>
<td>FeTiO₅</td>
<td>—</td>
</tr>
<tr>
<td>TiO₃</td>
<td>—</td>
</tr>
</tbody>
</table>

| Pseudobrookite | Fe²⁺ | Fe³⁺ | Ti⁴⁺ | Ti³⁺ | Reference |
| Fe₂TiO₅ | 4.48 | — | 1.28 | 3.52 | Virgo and Huggins (1975) |
| FeTiO₅ | — | 1.12 | 6.72 | — | Virgo and Huggins (1975) |
| Fe₂TiO₅ | — | 0.76 | 7.24 | — | Virgo and Huggins (1975) |
| FeTiO₅ | — | 3.80 | 4.20 | — | Virgo and Huggins (1975) |

**REFERENCES**

Grey and Ward (1973)

Navrotsky (1975)

Pedersen (1979)

Virgo and Huggins (1975)
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 (Mg,Mn,Ca)TiO$_2$ molecule are plotted to the right. Those minerals plotted above the FeTiO$_2$ to (Mg,Mn,Ca)Ti$_2$O$_3$ 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 (Al,Cr,V)$_2$(Ti,Zr)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 (Al,Cr,V)$_2$(Ti,Zr)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, 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 2a, 2b, 2c. 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 1a, 1b, 1b, 1b, 2, 2a, 3, 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, 5–7. Steele (1974): analyses 2a, 2b, 2c. 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.


from Mg$_2$Ti$_3$O$_7$ to Fe$_3$Ti$_2$O$_7$ and represents equal proportions of MgTiO$_3$ and TiO$_2$. 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$_3$Ti$_2$O$_7$ and a compositional range limited by FeTi$_2$O$_7$, FeMg$_{3/2}$Ti$_{1/2}$O$_7$, and compositions between these limits. Pseudobrookite is orthorhombic and in space group $Bbmm$. 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$_2$Mg$_{3/2}$Ti$_{1/2}$O$_7$ and a compositional range limited by Mg$_2$Ti$_3$O$_7$, FeMg$_{3/2}$Ti$_{1/2}$O$_7$, FeTi$_2$O$_7$, Mg$_{3/2}$Ti$_{1/2}$O$_7$, and compositions between these limits. Armalcolite is orthorhombic and in space group $Bbmm$. It has unit-cell parameters approximating $a = 9.743$, $b = 10.024$, and $c = 3.738$ Å.

**ACKNOWLEDGMENTS**

I am indebted to the national representatives of the IMA Commission on New Minerals and Mineral Names who have taken time to consider and approve these proposals. Comments from E. H. Nickel and D. H. Lindsley have significantly improved the manuscript. The figures were drawn by A. Lloyd.

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Navrotsky, A. (1975) Thermodynamics of formation of some compounds with the pseudobrookite structure and of the FeTi$_2$O$_5$-TiO$_2$ solid solution series. American Mineralogist, 60, 249-256.

Ottmann, J., and Frenzel, G. (1965) Der Chemismus der pseudobrookite
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$_2$O$_3$, Cr$_2$O$_3$, and V$_2$O$_5$ are put together to form R$_2$O$_3$. 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$_2$TiO$_2$ and R$_2$O$_3$:TiO$_2$. If $0 < x < 0.33$, the Fe is taken as Fe$^{2+}$, and formation of FeO$_2$TiO$_2$ leaves TiO$_2$ in excess, which is recalculated as Ti$_2$O$_5$(i.e., Ti$_2$O$_5$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$_2$TiO$_2$ and Fe$_3$O$_4$. This procedure is similar to that used by Pedersen (1979) and Kesson and Lindsley (1975) and is satisfactory for most analyses. The Fe$^{2+}$/Fe$^{3+}$ or Ti$^{4+}$/Ti$^{3+}$ distribution determined in this way can be calculated back to the initial analysis to find the wt% FeO and FeO$_2$ (or TiO$_2$ and Ti$_2$O$_3$). 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$^{2+}$. 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$_2$O$_3$-Mg$_x$Ti$_2$O$_5$ join. The analyses where ZrO$_2$ is large are also those where Ti$_2$O$_3$ is greatest. It is assumed here that Ti$_2$O$_3$-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$_2$TiO$_2$, (Mg,Ca,Mn)$_2$O$_2$TiO$_2$, and Fe$_3$O$_4$:TiO$_2$ or Ti$_2$O$_3$: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:2TiO$_2$ percentage is the percentage of the distance from Fe$_2$Ti$_2$O$_7$ to (Mg,Mn,Ca)$_2$TiO$_2$ along that axis, and the Fe$_2$Ti$_2$O$_7$ percentage is the percentage of the distance from Fe$_2$Ti$_2$O$_7$ to Fe$_3$Ti$_2$O$_7$. These two distances define a unique point in the lower half of the diagram; the same relation holds for the TiO$_2$ percentage in the upper half of the diagram. The third quantity, the Fe$_2$Ti$_2$O$_7$ percentage, could be plotted using contours parallel to the (Mg,Mn,Na)TiO$_2$ to Fe$_3$Ti$_2$O$_7$ 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**

<table>
<thead>
<tr>
<th>Wt%</th>
<th>Molecular proportion</th>
<th>R_2O_3-TiO_2</th>
<th>MO-2TiO_2</th>
<th>Ti left</th>
<th>FeO-2TiO_2</th>
<th>Fe_2O_3-TiO_2</th>
<th>Corrected analysis (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>TiO_2</td>
<td>64.13</td>
<td>0.803</td>
<td>0.051</td>
<td>0.412</td>
<td>0.340</td>
<td>0.266</td>
<td>0.074</td>
</tr>
<tr>
<td>Al_2O_3</td>
<td>5.18</td>
<td>0.051</td>
<td>0.051</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>MgO</td>
<td>8.31</td>
<td>0.206</td>
<td>—</td>
<td>—</td>
<td>0.206</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>FeO*</td>
<td>20.14</td>
<td>0.280</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>0.133</td>
<td>—</td>
</tr>
<tr>
<td>Total</td>
<td>97.76</td>
<td>0.803</td>
<td>0.051</td>
<td>0.412</td>
<td>0.340</td>
<td>0.266</td>
<td>0.074</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Molecular proportion</th>
<th>4 components (wt%)</th>
<th>3 components (wt%)</th>
</tr>
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<tbody>
<tr>
<td>FeTi_2O_5</td>
<td>0.133</td>
<td>28.67</td>
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<tr>
<td>Fe_2TiO_5</td>
<td>0.074</td>
<td>15.90</td>
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<tr>
<td>MO-TiO_2</td>
<td>0.206</td>
<td>44.47</td>
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<tr>
<td>R_2O_3-TiO_2</td>
<td>0.051</td>
<td>10.96†</td>
</tr>
</tbody>
</table>

Note: This analysis is specimen 74585 (Smith, 1985) 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. R_2O_3 = Al_2O_3 + Cr_2O_3 + V_2O_3. 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 Ti^4+ and plot the phase in the lower half of the diagram. (There is not enough TiO_2 to form only FeO-2TiO_2, which would require 0.560TiO_2.) Some Fe must be used up to form Fe_2O_3-TiO_2. Calculate this as follows:

molecular proportion of FeO = 0.280 (from above) - 2 × molecular proportion of FeO_2 |

and

molecular proportion of TiO_2 = 2 × molecular proportion of FeO + molecular proportion of FeO_2

Hence, molecular proportion of TiO_2 = (0.280 - 2 × molecular proportion of FeO_2) + molecular proportion of FeO_2 = 0.340 (from above). So molecular proportion of FeO_2 = 0.074 (gives 11.77 wt% FeO_2) 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**

<table>
<thead>
<tr>
<th>Wt%</th>
<th>Molecular proportion</th>
<th>Oxygen proportion</th>
<th>No. of anions</th>
<th>No. of cations</th>
<th>R_2O_3-TiO_2</th>
<th>MO-2TiO_2</th>
<th>Ti left</th>
<th>FeO-2TiO_2</th>
<th>Fe_2O_3-TiO_2</th>
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<tbody>
<tr>
<td>TiO_2</td>
<td>64.13</td>
<td>0.803</td>
<td>1.605</td>
<td>3.463</td>
<td>1.731</td>
<td>0.110</td>
<td>0.890</td>
<td>0.731</td>
<td>0.574</td>
</tr>
<tr>
<td>Al_2O_3</td>
<td>5.18</td>
<td>0.051</td>
<td>0.152</td>
<td>0.329</td>
<td>0.219</td>
<td>0.110</td>
<td>0.890</td>
<td>0.731</td>
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</tr>
<tr>
<td>MgO</td>
<td>8.31</td>
<td>0.206</td>
<td>0.206</td>
<td>0.445</td>
<td>0.445</td>
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<td>—</td>
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</tr>
<tr>
<td>FeO</td>
<td>9.55</td>
<td>0.133</td>
<td>0.133</td>
<td>0.287</td>
<td>0.287</td>
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</tr>
<tr>
<td>Fe_2O_3</td>
<td>11.77</td>
<td>0.074</td>
<td>0.221</td>
<td>0.477</td>
<td>0.318</td>
<td>—</td>
<td>—</td>
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<tr>
<td>Total</td>
<td>2.317</td>
<td>5.001</td>
<td>1.605</td>
<td>3.463</td>
<td>1.731</td>
<td>0.110</td>
<td>0.890</td>
<td>0.731</td>
<td>—</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Molecular proportion</th>
<th>4 components (wt%)</th>
<th>3 components (wt%)</th>
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</thead>
<tbody>
<tr>
<td>FeTi_2O_5</td>
<td>0.287</td>
<td>28.67</td>
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<tr>
<td>Fe_2TiO_5</td>
<td>0.159</td>
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<td>MO-TiO_2</td>
<td>0.445</td>
<td>44.47</td>
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<td>R_2O_3-TiO_2</td>
<td>0.110</td>
<td>10.96</td>
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</table>

Note: Calculation as example 1 (App. Table 1), but assuming that the Fe^3+/Fe^2+ or Ti^4+/Ti^3+ ratios are known and calculating to 5 oxygen atoms per unit cell.