

# Plotting Mineral Compositions on Compatibility Diagrams

## Level 2 Computing — Project 5:

### Project Abstract

This project is an example of data handling and data plotting of mineral analyses that you can obtain from the electron microprobe. The objectives are to derive the plotting parameters for a Thompson AFM diagram and to plot mineral analyses in this ternary diagram. In Project 5 you will:

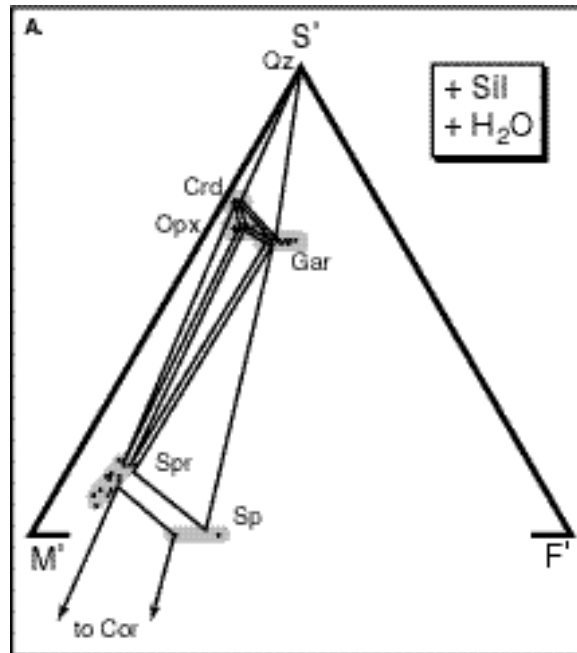
- (1) use EXCEL to determine the ternary coordinates of a Thompson AFM diagram (a muscovite, quartz and water projection),
- (2) calculate the AFM coordinates for several mineral assemblages,
- (3) plot these on a ternary diagram using DeltaGraph,
- (4) edit the DELTAGRAPH file in ILLUSTRATOR. You should produce **publication quality** figures.

You will be supplied with an EXCEL file with mineral formulas — download via the link in the Level 2 DIY Computing page.

Some of this material may be unfamiliar, but try to work through this with others in your year.

### Background

Probably all of you have seen ternary diagrams with mineral compositions plotted on them. Below is an example of this kind of diagram (from Kriegsman & Schumacher, 1999):



**Figure 4.** Representative compositions of cordierite (Crd), sapphirine (Spr), gedrite, orthopyroxene (Opx), spinel (Sp) and garnet (Gar) on a projection from sillimanite to the  $\text{SiO}_2\text{-MgAl}_2\text{O}_4\text{-FeAl}_2\text{O}_4$  plane of a  $\text{FeO-MgO-Al}_2\text{O}_3\text{-SiO}_2$  tetrahedron. Note that not all phases actually coexist with sillimanite.

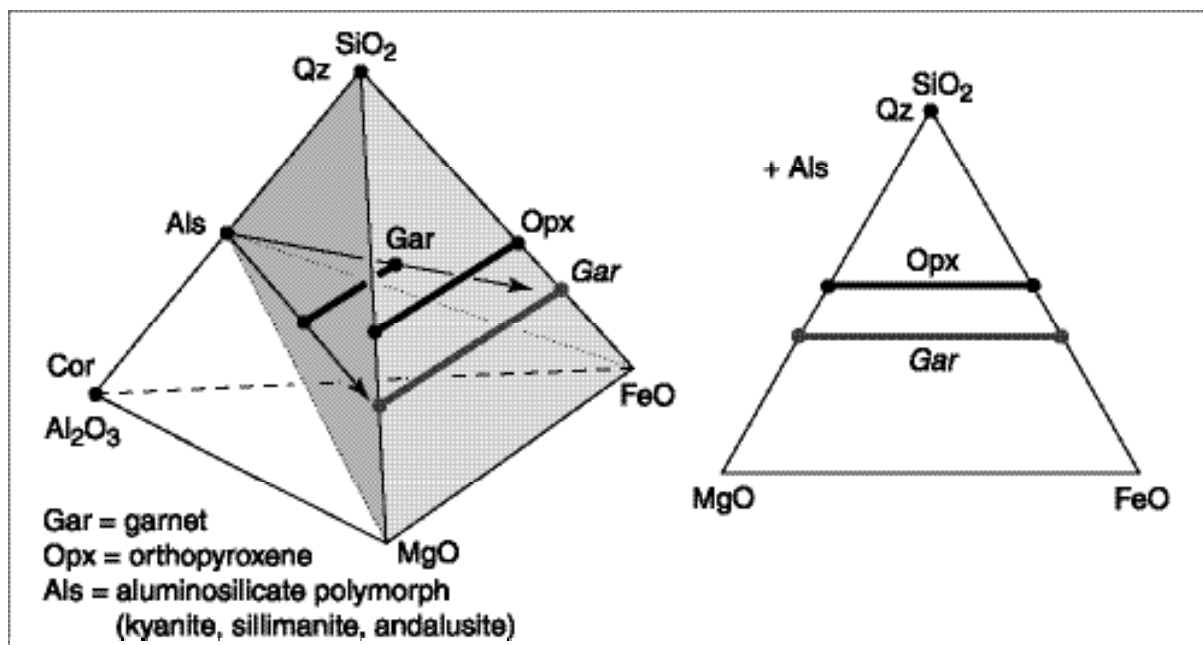
These kinds of diagrams portray two types of information: (1) the compositional ranges of all or most of the minerals (dots above) and, if the conditions of the diagram are met, (2) the compositions of coexisting minerals in stable assemblages (tie lines and triangles above). One advantage of this type of diagram is that the compositions of all or usually most of the rock-forming minerals can be summarized in a single diagram. When using these diagrams to compare assemblages, it is important that one plot only mineral compositions that formed at the same P-T conditions coexist with the excess phases (those indicated with a “+” above).

*So what are “excess phases”?*

The diagram above is a “projection” from water and the mineral phase sillimanite. By projection from various phases one can reduce the number of chemical components that need to be shown on the diagram. In the example above the “projection” from sillimanite eliminates the need to show  $\text{Al}_2\text{O}_3$ . What are the advantages of this? In this case, it means the minerals can be plotted on two-dimensional ternary diagrams, which are easier to visualize than 3-dimensional tetrahedral diagrams. The disadvantages is that not all assemblage can be shown (i.e., those without the projected phase should not be plotted when analyzing assemblages).

### Example: Projections and Transforming Components

Below is an example of the graphical basis of a projection from aluminosilicate (Als) onto the FeO-MgO-SiO<sub>2</sub> plane of an FeO-MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> tetrahedron. Fe-Mg garnet plots within the tetrahedron and orthopyroxene plots on the face of the tetrahedron that we are projecting to. Orthopyroxene will have the same position on the FeO-MgO-SiO<sub>2</sub> ternary, but the position of the garnet is only approximately known. With care and good graph paper, one could derive the plotting position of garnet on the FeO-MgO-SiO<sub>2</sub> ternary graphically. However, it is relatively easy to derive the coordinates of garnet mathematically.



Left: FeO-MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> tetrahedron showing projection of garnet to the FeO-MgO-SiO<sub>2</sub> plane. Right: the resulting ternary diagram.

The coordinates of garnet of the FeO-MgO-SiO<sub>2</sub> ternary are obtained by doing a **coordinate transformation**, which is no more than setting up a matrix and finding its inverse. The most difficult aspect of this operation is setting of the matrix properly. The **original coordinates** (corners) of the tetrahedron are FeO-MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>, but to project from Als onto FeO-MgO-SiO<sub>2</sub> we need a new tetrahedron with the corners FeO-MgO-Als-SiO<sub>2</sub>. The proper form of the matrix is shown below:

MATRIX					EXCEL function	INVERTED MATRIX				
	$S'$	$Als$	$M'$	$F'$		$SiO_2$	$Al_2O_3$	$MgO$	$FeO$	
$SiO_2$	1	1	0	0	do matrix inversion	$S'$	1	-1	0	0
$Al_2O_3$	0	1	0	0		$Als$	0	1	0	0
$MgO$	0	0	1	0		$M'$	0	0	1	0
$FeO$	0	0	0	1		$F'$	0	0	0	1

The inverted matrix indicates how the **new coordinates** are calculated:

$$S' = 1 SiO_2 - 1 Al_2O_3$$

$$M' = 1 MgO$$

$$F' = 1 FeO$$

$$Als = 1 Al_2O_3$$

Since we are projecting from **Als**, the value of this coordinate is ignored, which leaves us with the remaining three, **S', M', F'**.

You all know that pyrope garnet is  $Mg_3Al_2Si_3O_{12}$ , so for pyrope:

$$S' = 3 - 1 = 2$$

$$M' = 3$$

$$F' = 0$$

$$\text{Total} = 5$$

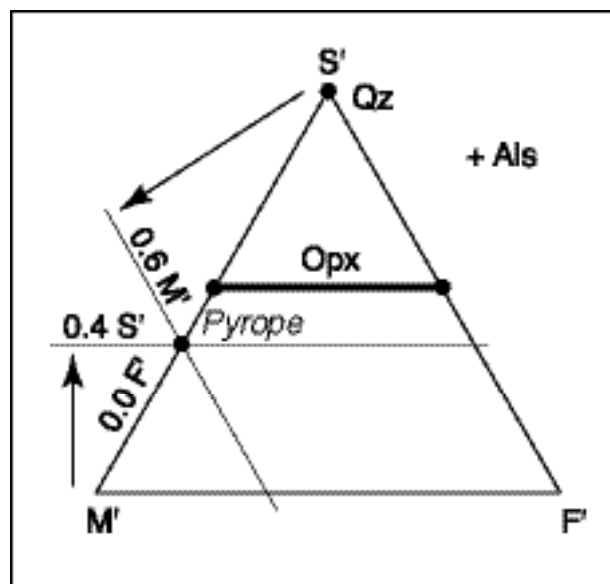
The ternary coordinates are:

$$S' = 2/5 = 0.4$$

$$M' = 3/5 = 0.6$$

$$F' = 0/5 = 0.0$$

The position of pyrope is shown below:



To perform a matrix inversion in EXCEL, use the general formula “=MINVERSE (array)”. To use this formula you must:

- (1) select location of the result (see below)
- (2) either use the menus to find and insert the formula (**Insert > Function...**) or type in “=MINVERSE(first cell : last cell)”.
- (3) press the **apple-enter** keys, which results in braces “{ }” around the formula:

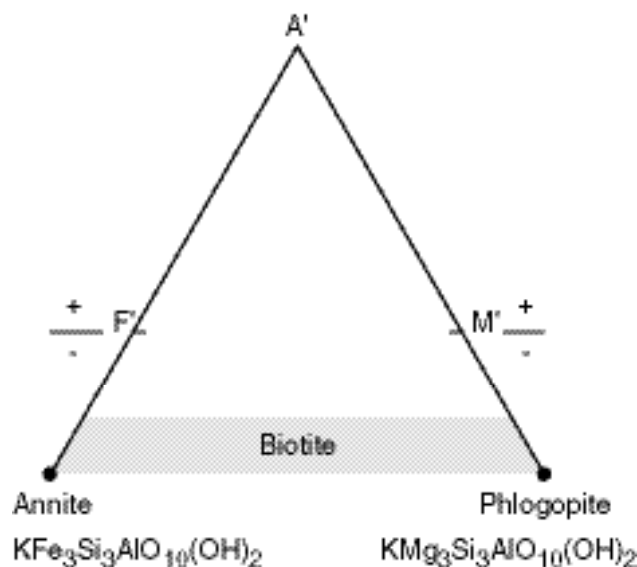
**apple-Enter**

	A	B	C	D	E
1		S'	Als	M'	F'
2	SiO <sub>2</sub>	1	1	0	0
3	Al <sub>2</sub> O <sub>3</sub>	0	1	0	0
4	MgO	0	0	1	0
5	FeO	0	0	0	1
6					
7					
8		SiO <sub>2</sub>	Al <sub>2</sub> O <sub>3</sub>	MgO	FeO
9	S'	1	-1	0	0
10	Als	0	1	0	0
11	M'	0	0	1	0
12	F'	0	0	0	1
13					

## Project 5

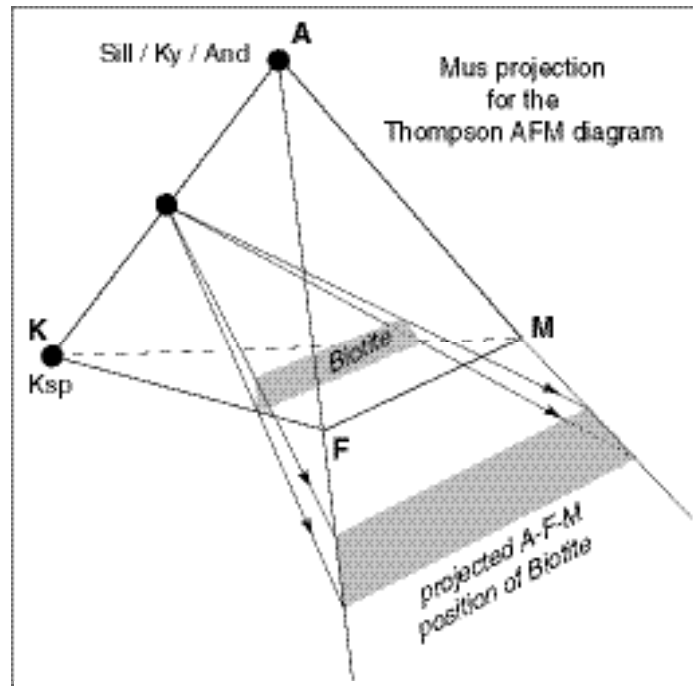
### Introduction

In your project you will plot several mineral compositions on a Thompson AFM diagram (a muscovite, quartz and water projection). The Thompson AFM diagram that you will use to plot the mineral compositions should look something like the one below with biotite plotting at negative A' component (below the base of the triangle—a line between F' and M'), all the other minerals that are common in pelitic rocks (garnet, staurolite, sillimanite cordierite) plot in the positive parts of the diagram.



The diagram is a schematic (FeO + MnO + ZnO) - MgO - Al<sub>2</sub>O<sub>3</sub> ternary diagram and is a projection from muscovite, quartz and water.

The diagram below illustrates the graphical projection of biotite onto the  $A' - F' - M'$  plane. The coordinates that you have calculated are for this 2-dimensional (triangular)  $A' - F' - M'$  plane.



As you may notice, biotite projects below the line between  $F'$  and  $M'$ . This means on a triangular Thompson AFM diagram biotite has negative Al!!!!. Is this possible? Yes it is. Any point that lies outside of the triangle will have at least 1 negative coordinate. Normally, we do not plot outside the bounds of triangular graph paper but there is no reason not to. Commercial computer graphics applications do not recognize negative ternary coordinates. Plotting these mineral compositions in DeltaGraph requires a little extra effort—this is the final part of this week's project.

### The assignment

You will need to do the following:

- (1) use EXCEL to determine the plotting parameters of a Thompson AFM diagram (a muscovite, quartz and water projection).
- (2) use the AFM diagram coordinates to calculate the AFM plotting positions of all the minerals in the data file (**data** sheet in **Proj5.xls**). Note these are real analyses, so there are additional elements. When plotting, ignore Ti, Ca and Na. Add Mn and Zn to Fe.
- (3) plot these on a ternary diagram using DeltaGraph,
- (4) edit the ternary in ILLUSTRATOR.

## The results

You will produce the following:

- (1) A labeled copy of your input matrix and its inverse (the **AFM Coord** sheet).
- (2) A labeled **publication quality** figure.

## Getting started

Below are brief instructions of the procedure. In additions to these instructions you will need to refer to the example described at the beginning of this document and to the instructions in the **Proj5.xls** workbook to complete the assignment.

(1) In your project you will need to calculate the **new coordinates** for a Thompson AFM projection from quartz, muscovite and water. To get you on the right track, the starting matrix should look something like this (see the **AFM Coord** sheet of the **Proj5.xls** workbook):

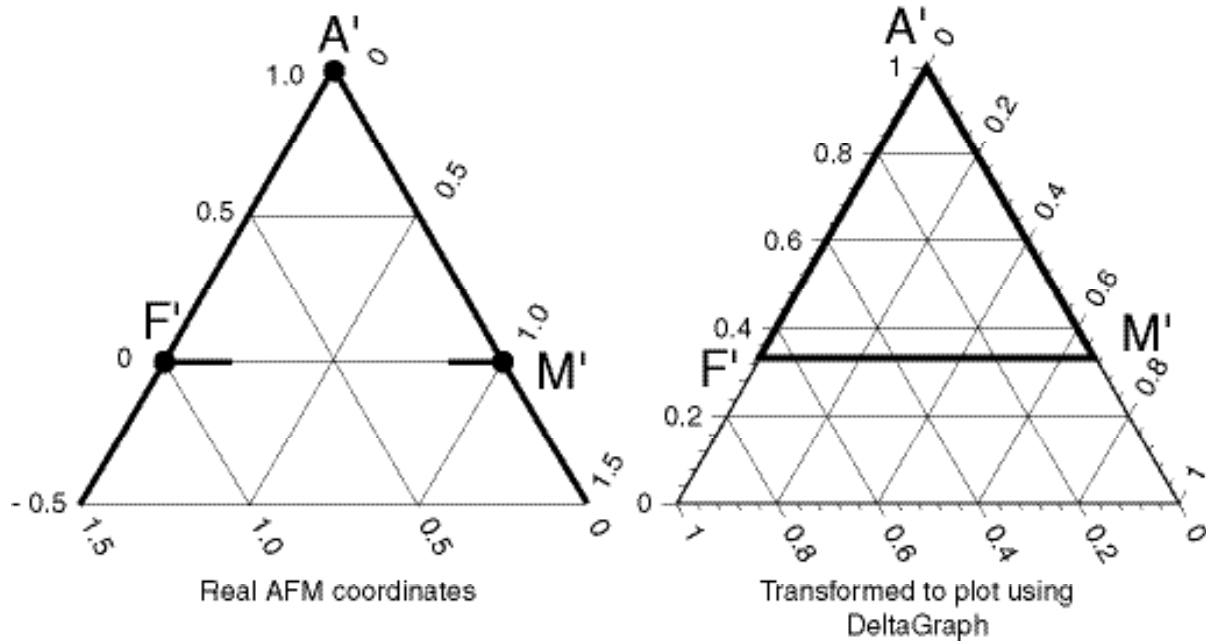
	<i>Qz</i>	<i>A'</i>	<i>F'</i>	<i>M'</i>	<i>mu'</i>	<i>W</i>
<i>SiO<sub>2</sub></i>						
<i>Al<sub>2</sub>O<sub>3</sub></i>						
<i>FeO</i>						
<i>MgO</i>						
<i>K<sub>2</sub>O</i>						
<i>H<sub>2</sub>O</i>						

To fill in this matrix, you will need to know the chemical formulae for water, quartz and muscovite, which is based on 12 (O,OH). Fill in the upper array in the **AFM Coord** sheet of the **Proj5.xls** workbook and do a matrix inversion (see Excel formulae) to obtain the values for the lower array.

The matrix inversion will yield values for all six of the new components, but you will only use the values for **A' - F' - M'**; since you project from **W, qz** and **mus**, their values (coordinates) are not used on the Thompson AFM diagram.

(2) Use the mineral formulae in the **data** sheet define an array consisting of **Si, Al, Mg, (Fe+Mn+Zn)** and **K**. Copy the **A', F',** and **M'** from the **AFM Coord** sheet then use these to sets of information to calculate the coordinates **A', F',** and **M'** for each mineral.

(3) As mentioned above, on the Thompson AFM diagram biotite will have a negative AFM coordinate. On triangular graph paper, it is easy (but not intuitive) to use negative values to plot points. You will need to convert the actual AFM coordinates into a set that can be used in Deltagraph.



In the DeltaGraph plot, annite should be located in the lower left corner and phlogopite in the lower right corner. **Hint:** you will need to know real AFM coordinates of annite and phlogopite on the diagram on the left. For the starting array, the “compositions” of **F'**, **M'** and **A''** equal the real AFM coordinates of annite, phlogopite and **A'**.

I hope you notice that converting the real AFM coordinates to DeltaGraph AFM coordinates is analogous to the procedure that was used to obtain the mineral AFM coordinates from the mineral formulae. Plot the minerals in DeltaGraph, export to Illustrator and make a proper AFM presentation of the data.

*Next year you will repeat a similar exercise in the Metamorphism course.*