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Frequency Distribution Of Pyroxene Types And A Method To Separate The Composition Of Multiple Pyroxenes In A Sample

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FREQUENCY DISTRIBUTION OF PYROXENE TYPES AND A METHOD TO
SEPARATE THE COMPOSITION OF MULTIPLE PYROXENES IN A SAMPLE

by

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ABSTRACT

Determining mafic mineral composition of asteroid bodies is a topic reviewed by M.J. Gaffey et al. (2002). The iterative procedure discussed can be implemented as an algorithm, and such efforts revealed weaknesses that are examined in this work. We seek to illustrate the limits of this method and graphically determine its predictions. There are boundaries in the formulae given where the equations break down. In ranges where mafic mixtures are predicted, a method is illustrated that allows a decoupling of these mixtures into the constituents.

For those who believe that obstacles make life impossible. It does. But doing the impossible is what makes it so much fun.

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CHAPTER 1: INTRODUCTION

Sometime in the middle of the 16th century Bode's Law was formulated. A law that at the time was thought to be a formula for the placements of planetary bodies in our solar system, showed a huge gap between Mars and Jupiter. With the general belief that Bode's Law was valid, this led to the idea that there was an as-of-yet undiscovered planetary body in an orbit between these two planets and so began a hunt to discover it.

This hunt continued for some time, and though not one planet was found something was in the gap. Floating debris known as asteroids peppered the region between Mars and Jupiter (among other places later discovered) and cataloguing them became a serious undertaking amongst certain astronomers. During the beginning, these asteroids were merely points of light in the sky. With the creation of better telescopes and cameras, the race began to try and capture higher resolution images of this debris.

Now there have been flybys of asteroids now with crisp images like that of 253 Mathilde by the NEAR spacecraft and asteroid Ida and its satellite Dactyl by the Galileo spacecraft. Also of interest is the Itokawa flyby with Hayabusa, scheduled to return sometime around 2010. The interest of course is in learning what makes up these objects and linking them to a more terrestrial resource available to us; meteorites.

Two important questions that can be asked when studying a meteorite include: What time period in solar system formation does the meteorite represent? Where (as in what orbit) does the meteorite come from? The second question is answered by linking meteorites with parent bodies and increases the spatial scope of our understanding of solar system history.

Determining the mineralogical characteristics of these asteroids provides a method to link meteorites to their parent asteroid bodies. This in turn hands the community a unique glimpse into the original composition of the solar system during the formation of planetesimals. While not all minerals have features in visible and VNIR spectra transition metal ions do. Common mafic minerals like those in the olivine and pyroxene groups are prevalent in chondrites and achondrites and show such spectral features. This forms a basis for attempts to determine the composition of asteroids using spectra.

When obtaining spectra from an asteroid, the first natural instinct was to compare them to the spectra library of the meteorite collection available on Earth. This had inherent problems making exact matches since the terrestrial collection is limited, but provided pretty good guesses about the surface characteristics of asteroids. So exact matches are nearly impossible (barring extreme luck) but it was possible to say that certain asteroids were “similar” to samples of meteorites.

The Gaffey et al (2002) method covers a method of determining the mafic composition on the surface of asteroids based on the location of two particular features in their spectra. These two bands location values are substituted into a series of iterative formulae until convergence is obtained. For the quantum mechanical background on this method refer to Burns (1970a,b, 1993), Adams (1974, 1975), Salisbury et al. (1975), Gaffey (1976), King and Ridley (1987), Gaffey et al. (1989), Cloutis and Gaffey (1991a,b) and Calvin and King (1997).

Gaffey et al. (2002) condenses this information into two sets of predictive formulae for pyroxene composition from a series of spectral measurements taken at room temperature.

There was a thought that these formulae could be used to map out potential classes of asteroids to attempt to see what potential discoveries lay in wait for the community using Gaffey's method. Since the formula sets were algebraic in nature plotting their results within appropriate boundaries would be elementary. This led to a series of questions about the validity of these formulae and revealed issues that this paper seeks to address.

In part 1 a brief introduction to the subject and to the formulae provided in Gaffey et al. (2002) will be made along with some highlights of the errors found. In part 2 the frequency distribution map predicted by the formulae will be discussed. This will lead to acceptable band numbers and their scatter plot in part 3. We also point out specific areas where the predictions either fail due to boundary conditions or get a little more complicated. In the case of mixed mafic compositions, it is shown that with the appropriate mappings available a decomposition of the components is possible. This presents an advance in the Gaffey et al. (2002) method that, ironically, is shown to produce questionable results.

CHAPTER 2: MAFIC MINERAL COMPOSITION

The pyroxene group is a well studied group of minerals found in igneous rocks. The group is categorized by a generic formula XYZ_2O_6 where the variables have a substitution list of acceptable ions and constructions rules for applicable combinations and or course their reduced forms. The importance of this mineral is that at high temperatures the crystalline structure begins to form. When asteroids cooled and since these minerals are spectrally observed, it is expected that crystallization occurred early on. This early crystallization gives us a glimpse not only into the formation of asteroids, but also if any materials were trapped in minor imperfections it hands the community a fantastic opportunity to study pristine material from the early formation of our solar system.

The particular mineral type referenced in Gaffey et al. (2002) is a combination of $CaSiO_3$ wollastonite (Wo) and $FeSiO_3$ ferrosilite (Fs). Studies of olivine-pyroxene mafic were first undertaken by Adams (1974, 1975), King and Ridley (1987) and Cloutis and Gaffey (1991a). The formulae presented by Gaffey et al. (2002) were derived from measurements made at room temperature. They use the centers of absorption bands to uncover the composition of pyroxene (molar Calcium(Ca) content [Wo] and molar Iron(Fe) content [Fs]).

The pyroxene combinations have documented effects on asteroid spectra as shown in figure 1. As olivine is added to the mix, features become more prominent as

opposed to spectra with mostly pyroxene which is flattened. This observation alone can provide an educated guess about the surface composition of other asteroids.

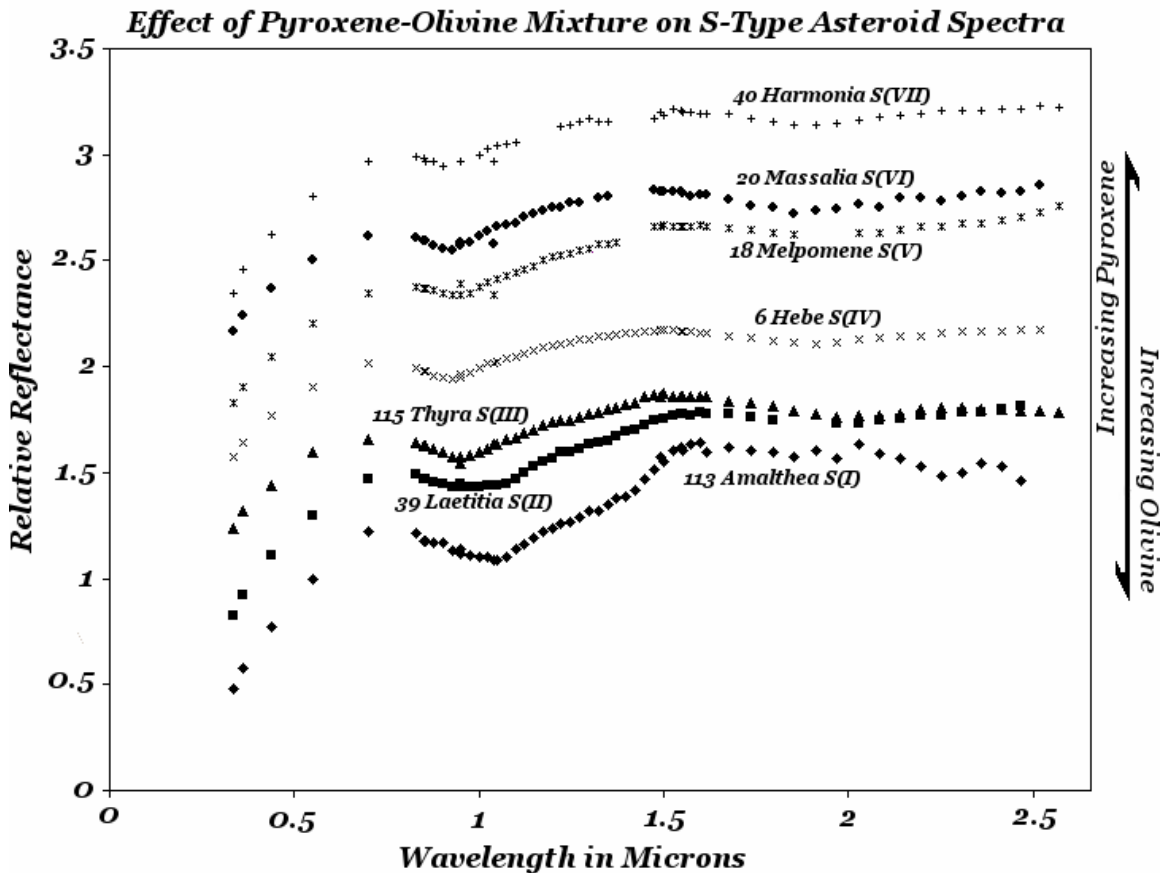


Figure 1: Effects of pyroxene-olivine mixtures on spectra of S-type asteroids. 113 Amalthea S(I) is mostly olivine while 40 Harmonia S(VII) is mostly pyroxene.

Gaffey et al. (2002) attempted to fit spectra observed on earth at room temperature to a set of formulae. The idea is to obtain the center of two bands (Band 1 and Band 2 ; see formula 1 and 2) and plugging them into one set of formulae. The resulting answer is then substituted into the second set and this process continues the answers begin to converge. The acceptable range of the centers of Band 1 is 0.9-1.07 μ m and those of Band 2 a range of 1.76-2.38 μ m.

$$W_o (\pm 3) = 347.9 \times \text{BI Center } (\mu\text{m}) - 313.6 \quad (F_s < 10; W_o \sim 5-35 \text{ excluded}) \quad (1a)$$

$$W_o (\pm 3) = 456.2 \times \text{BI Center } (\mu\text{m}) - 416.9 \quad (F_s = 10-25; W_o \sim 10-25 \text{ excluded}) \quad (1b)$$

$$W_o (\pm 4) = 418.9 \times \text{BI Center } (\mu\text{m}) - 380.9 \quad (F_s = 25-50) \quad (1c)$$

$$F_s (\pm 5) = 268.2 \times \text{BII Center } (\mu\text{m}) - 483.7 \quad (W_o < 11) \quad (2a)$$

$$F_s (\pm 5) = 57.5 \times \text{BII Center } (\mu\text{m}) - 72.7 \quad (W_o = 11-30, F_s < 25 \text{ excluded}) \quad (2b)$$

$$F_s (\pm 4) = -12.9 \times \text{BII Center } (\mu\text{m}) + 45.9 \quad (W_o = 30-45) \quad (2c)$$

$$F_s (\pm 4) = -118.0 \times \text{BII Center } (\mu\text{m}) + 278.5 \quad (W_o > 45) \quad (2d)$$

The restrictions denote values unseen naturally according to Deer et al. This iterative procedure is quite insensitive to which formula one starts with. This is due to the very consistent values the 1a, 1b and 1c return. For example, from 1.03-1.07 μm the W_o result always requests the use of 2d. Therefore no matter what F_s answer is returned, the result of any formula chosen will return you to 2d again.

Regions in the first three formulae that act like this are 0.9-0.931 μm (redirects only to 2a), 0.934-0.978 (redirects only to 2b), 0.987-1.013 μm (redirects only to 2c), and 1.03-1.07 μm (redirects only to 2d). So using a 0.001 increment, ~83% of the values returned by all three formulae in set 1 (1a, 1b and 1c) only point to one of the members in formulae set 2. This behavior immediately leads to an answer in three iterations.

The first region is where all of the negative errors occur in the Wollastonite formulae (see figure 2). This always points to 2a in the Ferrosilite set, the formula where

the majority of negative error and greater than 100% error is found (see figure 3). This creates a large gap when comparing Gaffey predictions with empirical data.

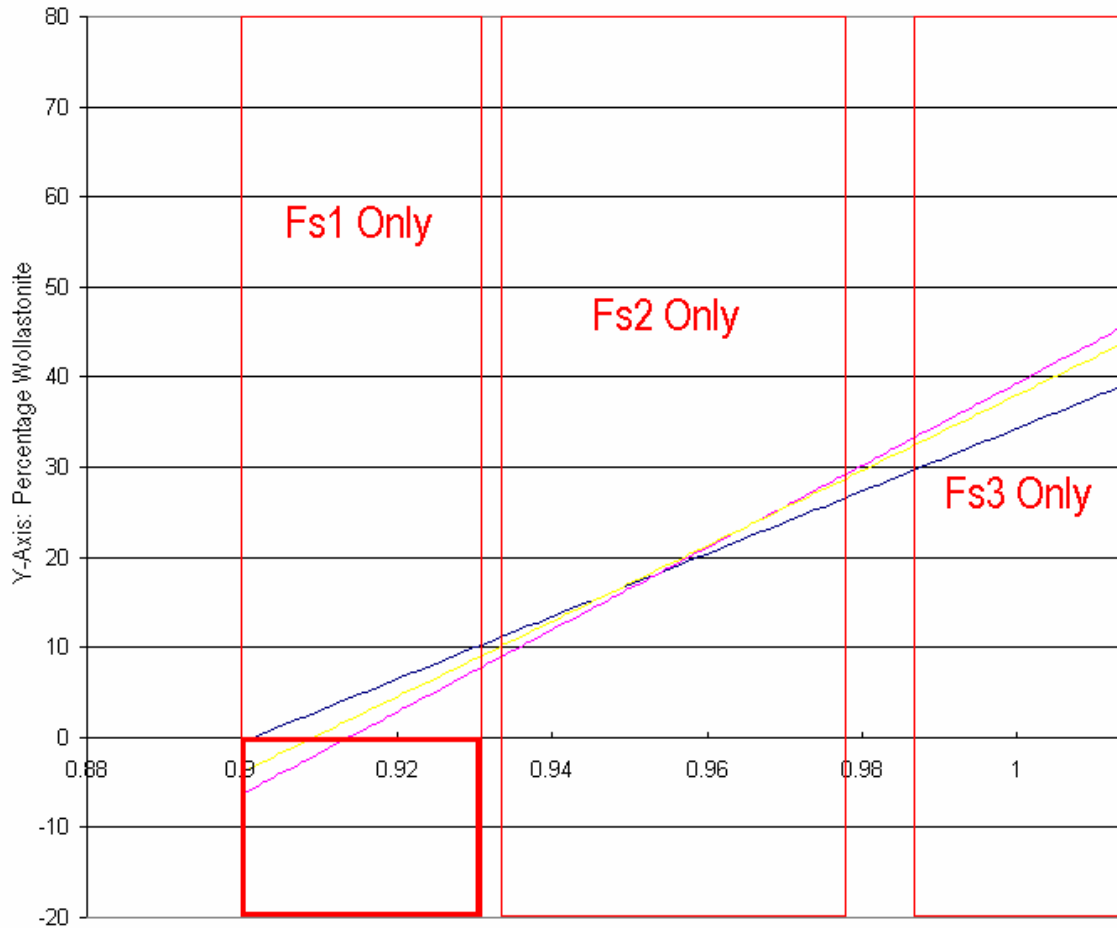


Figure 2: A plot of the Wollastonite set. The formula set points as a group to certain members of the Ferrosilite set. Note that all of the negative error is in a region that points only to the first Ferrosilite formula in ~0.9 – 0.93 μ m region.

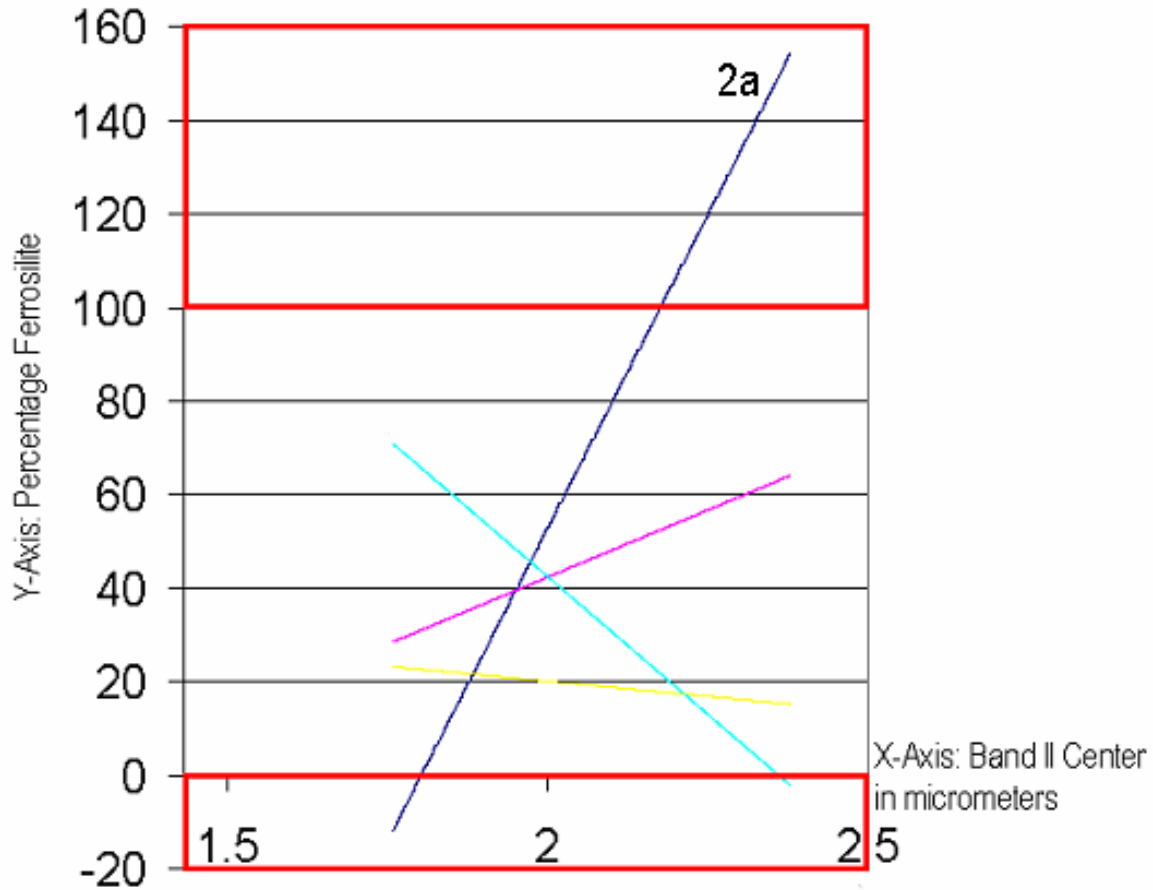


Figure 3: A plot of the Ferrosilite set. Note that almost all of the error is in 2a, the formula that all of the negative error Wollastonite formulae point to. This causes the large unphysical gap in figure 6.

The rest of the regions (0.932-0.933 μm , 0.979-0.986 μm and 1.014-1.029 μm) are transition regions that point to two members of set 2. An example of this is the region from 1.014-1.029 μm the W_o result ships you to either 2c or 2d. This automatically excludes 2a and 2b from consideration. When this is case, convergence on the answer is only a matter of returning to one of the set 2 formulae for the second time and then the pattern obtained repeats itself. For example let Band 1 be 1.016 μm and Band 2 be 2.04 μm . Starting with 1a, one obtains the following iteration: $W_o40 \rightarrow F_s20 \rightarrow W_o47 \rightarrow F_s38 \rightarrow W_o45 \rightarrow F_s20$ and the pattern goes from there.

Gaffey et al (2002) shows no method of determining if the pyroxene pairs are Fs20:Wo47;Fs38:Wo45 or Fs20:Wo45;Fs38:Wo47. Without a mapping of predicted acceptable values determining this proves difficult. There are no regions within the limits that point to three formulae in set 2. Stability in the formulae are a direct result of eliminations occurring in set 2.

There are also mathematically ambiguous regions in the formula. Gaffey et al. (2002) mentions that obtaining a value of Wo11 creates a branching effect that may show either Fs30 or Fs37. This does not appear to be the case. If one looks at the restrictions in (2a) and (2b) they are not linked in any way. Starting with each formula; it can be shown that they all converge at the same values.

While it seems that the Wo11 problem may have been erroneously mentioned, no mention of problems occurring when Wo25 or Fs30 are obtained is made. In the final formula (2d) the calculation first obtains Fs53 and is not permitted by the formula. Gaffey et al. (2002) continued the calculation despite this.

CHAPTER 3: FREQUENCY DISTRIBUTION PREDICTIONS

The formulae should predict the possible types of composition we should find in asteroid bodies. Code was written to determine the pyroxene composition in increments of $0.001\mu\text{m}$, assuming that the centers of Band 1 has an acceptable range of $0.9\text{-}1.07\mu\text{m}$ and those of Band 2 a range of $1.76\text{-}2.38\mu\text{m}$.

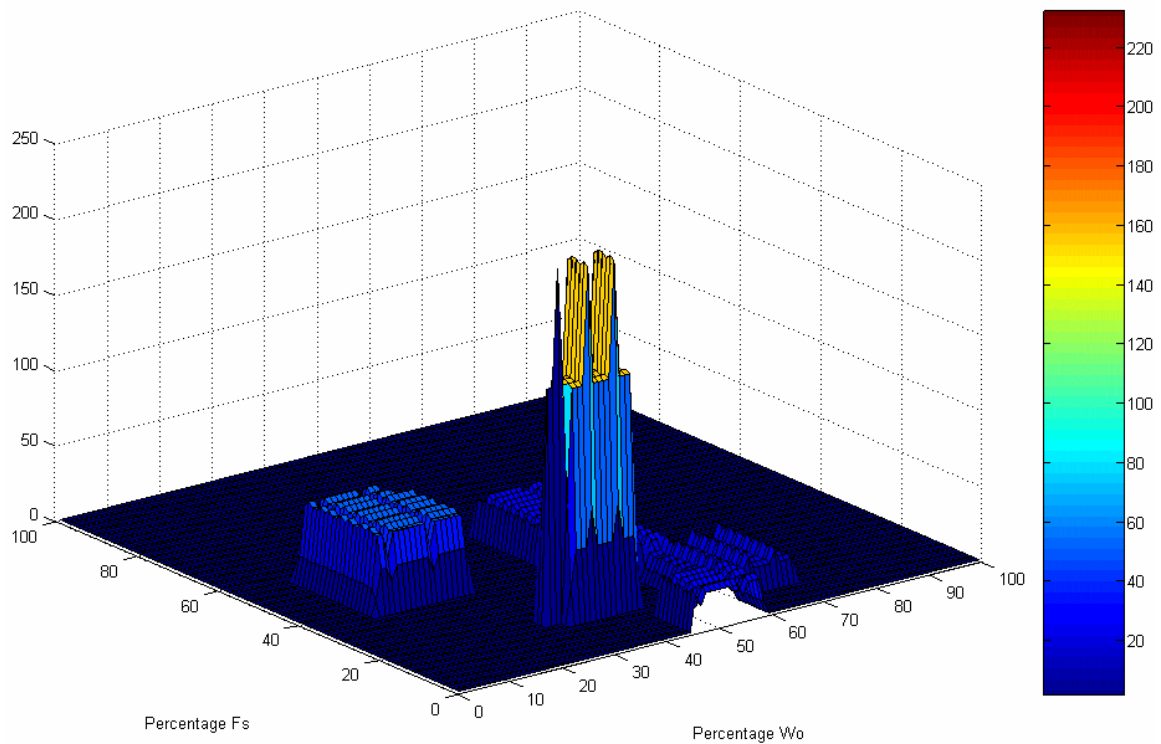


Figure 4: The frequency distribution map of pyroxene composition predicted by the Gaffey et al. (2002) formulae. The z-axis represents the number of times a particular combination of pyroxene was obtained.

The results of the code are seen graphically in Figure 2. The most abundant combination is heavily weighed in favor of a group of pyroxene compositions having

Wo~30-45 and Fs~15-23 with less populated (but larger) groups around them. These groups are surrounded by non-existent predictions and thus could be utilized to predict most likely compositions of asteroid pyroxenes.

Looking at Figure 3 for an overhead view of this distribution it is seen that there are five discrete groups of pyroxene. Anything above the diagonal line shows values predicted that are greater than 100%, clearly impossible.

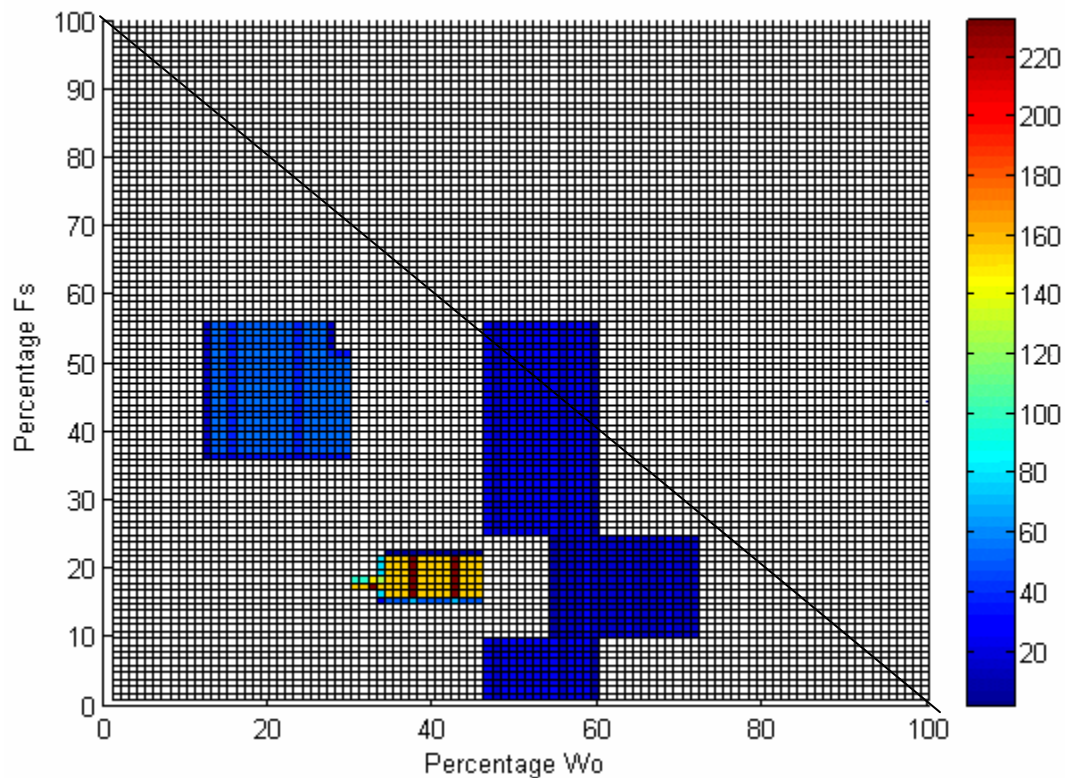


Figure 5: The overhead view of Figure 2, showing 5 distinct groups predicted by the Gaffey et al. (2002) formulae. The black diagonal line shows values that added together constitute a Wo:F_s combination whose sum is greater than 100%.

There were certain values returning single pyroxene compositions less than 0, also impossible. Other values of Band 1 and 2 also seem to predict multiple types of pyroxene. The validity of such predictions should be tested experimentally.

CHAPTER 4: ACCEPTABLE RANGES FOR BAND I AND BAND II

The Band 1 and Band 2 value ranges were pulled from Figure 5 of Gaffey et al. (2002) and shows band centers for pyroxenes done by Adams (1974) and Cloutis and Gaffey (1991a) in H, L, and LL chondrites. Filtering out unacceptable (less than 0% or greater than 100%) and plotting acceptable regions in the bands shows that there are gaps (see Figure 4) where observed data appears in zones where the formulae fail to produce reasonable answers.

Figure 4 is broken up into five regions (labeled 1-5). Region 1 represents Band values where the formulae 1 and 2 return answers that are discounted. This region also contains a large (and densely packed) cluster of observed data. Eliminations of the calculation were made based on strange behavior in the formulae that tended to cast doubt on any obtained composition. Behaviors included compositions less than 0%, greater than 100%, single branches that failed to converge and different branches returning different answers not of the multiple pyroxene type discussed in Gaffey et al. (2002).

For example at $\sim 0.92\mu\text{m}$ for band 1 and $\sim 1.79\mu\text{m}$, starting with any formulae in formula set 1, one obtains $\text{Wo}(6)$, $\text{Wo}(3)$ and $\text{Wo}(4)$ from 1a, 1b and 1c respectively. The appropriate choice is therefore 2a, returning $\text{Fs}(-4)$ and the cycle converges to $\text{Wo}(6):\text{Fs}(-4)$. Another example is at $\sim 0.925\mu\text{m}$ for band 1 and $\sim 1.87\mu\text{m}$ for band 2. Convergence is obtainable for all the formulae except if one starts with 2d and this returns an $\text{Fs}(58)$ and stops, there is no member of formulae set 1 that accepts this condition. For band 1 of $0.931\mu\text{m}$ and band 2 of $2.2\mu\text{m}$ the answers returned are $\text{Wo}(10):\text{Fs}(106)$, $\text{Wo}(9):\text{Fs}(106)$

and Wo(9):Fs(106) representing the greater than 100% composition errors. Even under the most lenient errors allowed by the formulae, -4 and -5 the answer Wo(4):Fs(101) shows no improvement.

Region 2 and 4 return acceptable converging answers with single compositions. Care had to be taken to evaluate the branches to avoid answers containing branches with similar answers. Observed data within region 2 and 4 is not as dense as in region one. Some eliminations were avoided based on the errors allowed such as 0.96 μm for band 1 and 1.9 μm for band 2. These returned normal values that converge on Wo(21):Fs(37). 2d however has a problem, it returns an answer of 54 and is thus excluded from any member of formula set 1. The error in 2d however is ± 4 and so barely slips into 1c if the answer is given the benefit of the doubt. Note the difference from the example in region 1, where 58 is excluded completely and the error was unable to keep it from being eliminated.

In region 3 of figure 4 multiple pyroxene compositions begin to appear as discussed by Gaffey et al. (2002) in section 3.3.3. These multiple pyroxene answers could not be separated into their components until the frequency map (figure 3) was created. Using this map it is now possible to determine which of the pyroxene combinations are available.

Using the point in figure 4 highlighted by the arrow in region 3, band 1 has a value of 1.018 μm and band 2 a value of 2.350 μm one can calculate a non-converging path which alternates between four values, a multiple pyroxene composition.

The path Wo41 \rightarrow Fs16 \rightarrow Wo48 \rightarrow Fs1 \rightarrow Wo41 can be calculated and loops around again giving four possibilities; Wo(41), Fs(16), Wo(48), Fs(1) in some unknown configuration. The question now is what are the individual pyroxene compositions

present in this calculation? The combinations are Wo(41):Fs(16), Wo(48):Fs(16), Wo(41):Fs(1) and Wo(48):Fs(1).

By looking at these combinations and comparing them to the groups in figure 3, one can see that certain compositions never show up and can thus be reasonably ignored. Using figure 3, one can separate the compositions of pyroxenes into Wo(41):Fs(16) and Wo(48):Fs(1).

Wo(41):Fs(1) is highly unlikely.

Wo(41):Fs(16) has a higher probability, occurring within the peak group.

Wo(48):Fs(1) is also possible and does occur on the map with some frequency.

Wo(48):Fs(16) is highly unlikely.

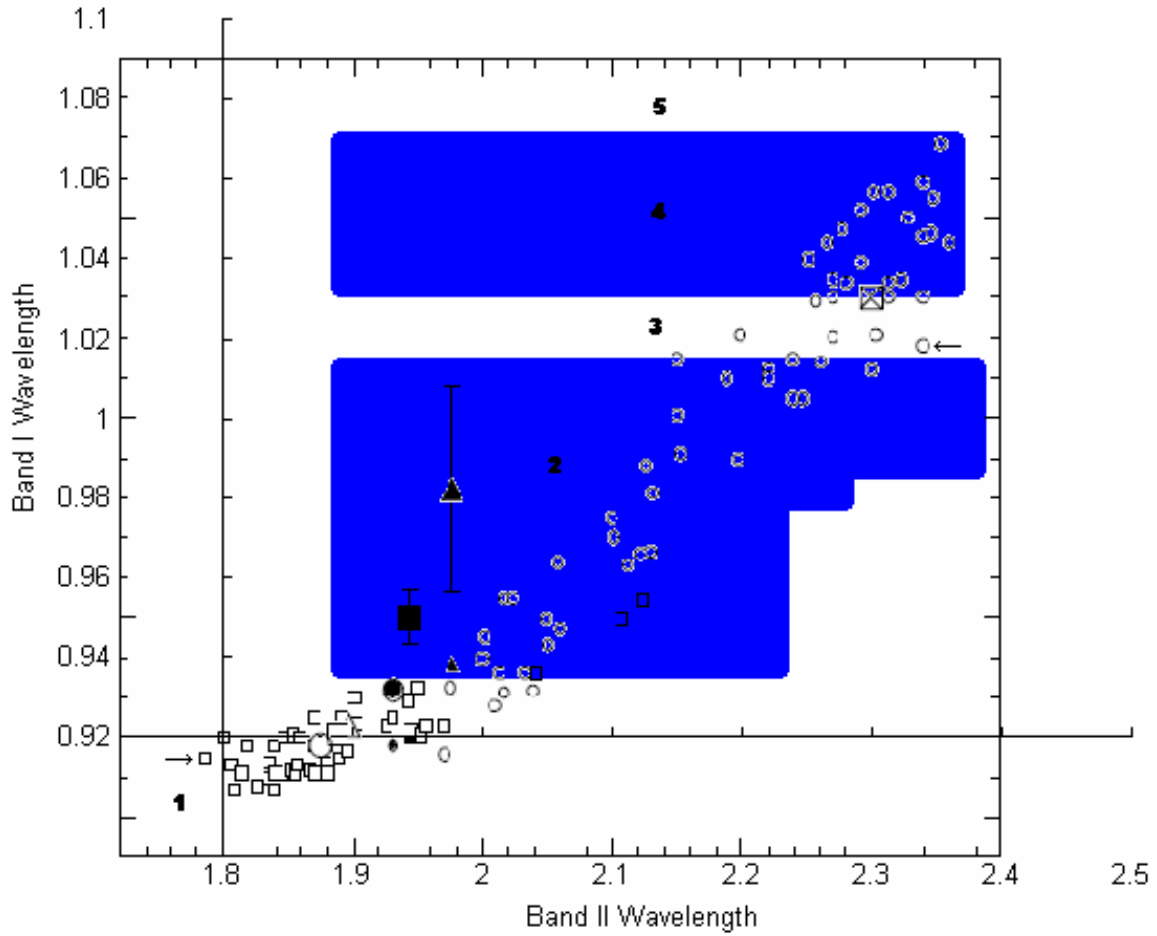


Figure 6: The dark region shows where acceptable compositions were obtained by Gaffey et al. (2002) while any other region returned unacceptable compositions (less than 0% or greater than 100%). A considerable amount of data is in the unacceptable regions.

CHAPTER 5: CONCLUSIONS

The pyroxene determination method used by Gaffey et al. (2002) lends itself to easy computer analysis. There are problem regions in the formulae given that need to be better understood. While the possibility of separating multiple pyroxenes was previously though impossible, it was shown that there is a way to extract acceptable values from a frequency map. Comparing the observed data to the method shows that the formula sets are lacking, especially in region 1 where a dense amount of observed points are predicted to have unacceptable compositions.

Future work will include a detailed analysis of all of the regions in figure 4. In Region 1, reasons why strange values are found should be sought out and corrected. Constraints for values to be accepted will be relaxed, since preliminary work has shown to produce micro regions of “almost acceptable” values. This may illuminate reasons why failures under strict rules occurred. Further experimental tests should be done to verify the results predicted in this work and Gaffey et al. (2002). Similarly, in regions 2 and 4, rules will be tightened to cause micro regions of “near failures.” In Region 3, a study of the kinds of pyroxene mixtures obtained will be done, detailing the composition types present and the number of pyroxene types present.

If a meteorite has a Band I and II feature that indicates two or more pyroxene types the chances of linking that meteorite to a specific asteroid or even a class of asteroids increases.

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