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# Automated Spectral Identification of Materials Using Spectral Identity Mapping

Robert William Cannon  
*Cleveland State University*

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AUTOMATED SPECTRAL IDENTIFICATION OF MATERIALS USING  
SPECTRAL IDENTITY MAPPING

ROBERT WILLIAM CANNON

Bachelor of Science in Chemistry

Cleveland State University

May, 2006

Submitted in partial fulfillment of requirements for the degree

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This Thesis has been approved  
for the Department of CHEMISTRY  
and the College of Graduate Studies by

---

Thesis Chairperson, Dr. John Turner

Chemistry \_\_\_\_\_  
(Department & Date)

---

Dr. Andrew Resnick

Physics \_\_\_\_\_  
(Department & Date)

---

Dr. Petru Fodor

Physics \_\_\_\_\_  
(Department & Date)

## **DEDICATION**

I would like to dedicate this thesis to my family and friends. They have supported me through my graduate education. Thank you for your support and letting me spend a significant amount of time away from you all to earn education.

## ACKNOWLEDGEMENTS

I sincerely thank Dr. John F. Turner II for his patience, time and guidance as my research advisor. I think that it is rare to work with those who have foresight and the ability progress based on their visions. I would also like to thank the members of my committee for their review of this thesis. The members were Dr. Petru Fodor and Dr. Andrew Resnick.

I would like to thank the Department of Chemistry for the opportunity to be a graduate in Master of Science in Chemistry program. I would also like to thank my classmates and co-workers that have assisted me with many aspects of my work.

I would also like to thank the generosity of a great many people who have contributed to this work through their previous accomplishments in securing samples, acquiring spectra, developing software tools, and lending their expertise to the greater goal of expanding knowledge about minerals, Raman analyses, database development, software, and multivariate methods. The work described in this thesis would not have been possible without contributions from many persons in the greater community, beyond Cleveland State University. The work presented here extends their efforts as well as previous work by Dr. Turner and his students, and makes use of pre-existing mineral spectra, instrumental methods, and multivariate strategies to provide what is intended to be a publicly accessible Raman database of mineral spectra. Ramindex is a trademark of Dr. Turner, under whose direction this work was performed.

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**ABSTRACT**

With increased use of Raman spectroscopic instrumentation for material analysis there has also been an increase in the amount of acquired Raman spectral data. Because of this, there is a clear need to develop and implement advanced spectral analysis techniques. This is especially true in cases where limited reference data may be available and large data sets need to be interpreted.

Raman spectral analysis and standardization techniques, along with a foundation for a comprehensive repository of Raman spectral data, will be described in this thesis. The main focus will be automated analysis and standardization of Raman spectral data using spectral identity mapping (SIM). In addition, details on how to promote widespread access to the analyzed data and SIM techniques will be given.

SIM, a statistical spectral analysis method, is useful as either a stand-alone data classification method or as a factor analysis step that precedes other multivariate approaches. SIM for calibrating spectra utilizes multivariate processing algorithms that can differentiate spectra according to the intrinsic nature of their spectral shapes. SIM also enables spectral identity mapping to be performed on unknown samples by calculating a set of scores giving the most likely match for given set of spectral information.

A SIM database of calibrated spectra and a proposal to utilize SIM matching algorithms via the internet was developed. There are currently few searchable databases available for Raman spectral data. Also, while there are many internet platforms available to publish spectra, some can be difficult to implement and most do not provide data to users in a way that is educational, engaging and fully oriented to the Raman community.

The software libraries given here provide a set of tools for data-basing, searching and interpreting spectral data while encouraging user/client participation in order to grow the spectral libraries. The hope is that the SIM results and the database developed here will promote SIM for more extensive use in future Raman spectra analyses as well as other forms of spectral data analyses.

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## CHAPTER I

### INTRODUCTION

Raman spectroscopy as a material analysis technique has become increasingly widespread due to the growing availability of affordable instruments. With the increase in acquired data it can be difficult to properly compare datasets due to differences in the instruments and the analysis techniques used. There are also challenges analyzing the data due to intrinsic spectral features such as variations in peak intensity ratios due to factors such as laser polarization and sample orientation. Other challenges include fluorescence and non-uniform baselines. Acquisition of large datasets presents the challenge of analyzing all of the data rapidly. Even though the Raman modality, including Raman imaging, is growing due to the wider availability of instrumentation, more efficient methods for data analysis are needed to rapidly characterize the vast sets of data being produced.<sup>1</sup>

The above problems are exacerbated by the fact that there are few web-accessible platforms that exist as spectral reference libraries for Raman data. One of these, the RRUFF<sup>TM</sup> project, with just over 3000 spectra is a typical web based information store and the majority of the materials are mineral samples.<sup>2</sup> Some spectral

databases such as GRAMS<sup>™</sup>, Bio-rad<sup>®</sup> and ICDD<sup>®</sup> request payment for use of their software and services.<sup>3-5</sup>

Overall, solving these problems requires large amounts of time for data processing due to the aforementioned issues. The time required can also lead to additional problems during data processing in the form of analyst errors. Hence, robust approaches are needed for automated analyses.

Spectral identity mapping (SIM) is a data reduction method which generates a score based on spectral shape.<sup>1</sup> SIM reduces the amount of a priori information needed and was initially designed to provide pseudo-color image contrast from hyperspectral data. SIM has shown significant ability in assisting with the analysis of spectral data individually and en masse; large scale analyses are achieved by integrating SIM based multi-spectral algorithms into automated spectral analyses.

Some additional features of SIM have been previously demonstrated by Turner et al.<sup>1</sup> in the analysis of various imaging data. Turner et al. showed that SIM provides enhanced chemical contrast for qualitative analysis and explain that SIM has quantitative potential.<sup>1</sup> The analytical properties demonstrated by SIM can be used with Raman spectroscopy to provide insightful data analysis and has the potential to be utilized across many fields where more powerful analytical techniques are needed. A list of some potential fields and sample types are given in Table I.



**Table I: Raman Applications with SIM**

Scientific Fields and Sample Types	
Pharmaceuticals	Biomaterials
Minerals	Advanced Materials i.e. Semiconductors
Forensics	Narcotics
Explosives	Archeology
Space Exploration	Coatings

Materials in these areas may contain complex heterogeneous samples that may be difficult or impossible to non-destructively analyze by other techniques. SIM is considered a chemical imaging technique that can be used to help determine chemical composition or to differentiate between spectra that have different shapes. Hence, SIM is particularly useful in data mining applications for existing databases and for developing new databases for biological materials. Many groups are acquiring data, but there are very few comprehensive electronic resources available for referencing and rapid evaluation of unknown materials based on their Raman spectrum.

One important application of Raman data mining is law enforcement. Accurate and rapid analysis of materials in this field can be critical to an investigation and have imminent life or death consequences. Biological, organic and inorganic materials are encountered in the field. In recent years there has been a new and growing reliance on Raman spectroscopy for chemical analyses using portable Raman spectrophotometers. This need has been stressed by Eckenrode et al.<sup>6</sup> stating, “Although there has been a great deal of progress in bringing Raman spectroscopy to the field, there remain several

areas where improvements and/or further testing are warranted. The data system (including the software and library-searching capabilities) will need to improve both in terms of the user interface and the library-search algorithms. A group frequency searching and screening capability would be highly desirable.”

In this project SIM is effectively used to develop a calibrated database of Raman spectra for spectral analysis. SIM enabled efficient calibration of over 1000 spectra saving a significant amount of time processing data one spectrum at a time. Using SIM reduces the likelihood of processing error while rapidly standardizing large data sets.

Additional aims were to develop user non-assisted data calibration and analysis algorithms, spectral identification algorithms with hyperspectral imaging capabilities and to produce efficient databasing and search algorithms that can be easily accessed through the internet. This was accomplished using original SIM computer algorithms written in Matlab<sup>®</sup>. Efficient calibration and analyses were achieved due to the flexibility of matrix based data handling methods. In order to make the data widely available over the internet, a combination of internet development libraries were used.

## **1.1 Statement of the Problem**

Raman spectroscopy is well suited for sample analysis in a many fields because it is a non-destructive technique that is chemically specific and requires little or no sample preparation. Many Raman modalities exist, exploiting many aspects of Raman spectroscopy including surface enhanced Raman scattering (SERS), coherent anti-Stokes Raman spectroscopy (CARS) and resonance Raman spectroscopy. There are other spectroscopic techniques available such as reflectance spectroscopy, x-ray diffraction,

x-ray fluorescence and polarizing microscopy for chemical identification, but these methods can require extensive data processing, sample preparation or are destructive. In some case, such as molecular UV-Visible absorption spectroscopy, the methods are not chemically specific.

One of the challenges in assembling a functional Raman database is in generating automated methods for performing spectral calibrations and spectral matching. Existing spectral analysis methods are not sufficient because they can rely on well defined spectral features and known chemical components.

Also, sample classes containing similar materials can exhibit either very different spectra or, conversely, similar spectral shapes to other sample classes leading to unclear results. In these cases an analysis can rely heavily on the analyst to properly interpret the spectra. This leads to a loss of a significant amount of time by the analyst. There is also an increased likelihood of processing error.

Most multivariate analyses rely on training data. There can often be unexpected and therefore unidentified constituents.<sup>1</sup> Complex sample mixtures that are typical for biological and mineral samples usually prevent the development of suitable training data that would assist with an analysis.

Additional problems can arise as a result of differences in instrument hardware and optical configurations. The problems with wide ranging system configurations are that aberrations from individual systems can occur anywhere from the source to the detector. Correlating data from different systems can also be difficult due to the spectral ranges of the sample data.

Spectral variations can manifest as peak shifting, independent wavelength ranges, baseline changes and potential artifacts. Artifacts can be recognized and

removed by trained analysts. Baseline changes or dark counts can be removed by subtraction. Peak shifting can be accounted for by employing a known standard for peak calibration adjustment. However, selecting the proper correction techniques for individual labs can be challenging due to these acquisition variations, spectral ranges and sizes of data sets.

### **1.1.1 Raman Spectroscopy in the Field**

Raman spectroscopy in the field presents its own set of challenges.

Improvements are needed to obtain enhanced S/N for portable Raman systems by the reduction in background signals from the environment and sample fluorescence.<sup>6</sup>

There have been attempts to solve this by utilizing longer wavelengths to reduce fluorescence and shorter wavelengths for increased scattering.

One important issue for field-portable Raman systems is the user interface.<sup>6</sup>

Software for field instruments can require several steps and extensive training.

Software control of library searches is also an area where further research and improvement is required. Several additional questions regarding software capability and analytical specificity are given by Eckenrode et al.<sup>6</sup>

### **1.1.2 Data Challenges**

Once properly processed and calibrated data sets have been developed, they can be difficult and expensive to make widely available to the public. In order to make analysis techniques and data widely available quickly, network software applications are required.

There are many computer program language choices available for algorithm development. Independent software development and utilization can be daunting for novice and experienced developers. Some development packages do not offer a full scope solution for delivering analytical methods and results in a meaningful manner. Purchased software can be difficult to utilize, implement to existing systems, and costly. Difficulties arise because some groups require specific data processing methods that fit their own needs as well custom graphical user interface (GUI) arrangements. For example, Eckenrode<sup>6</sup> states that the Federal Bureau of Investigation (FBI) requires customized databases for the samples they handle.

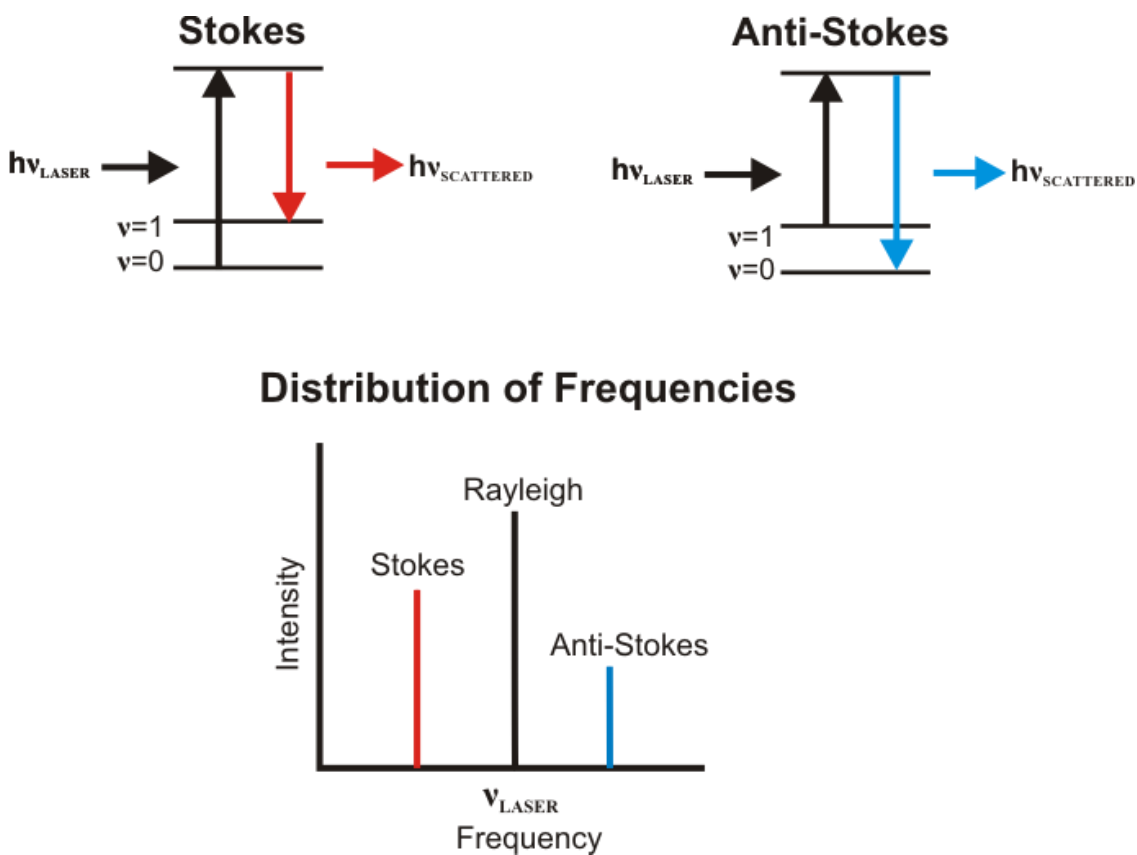
The research here focuses on the development of robust automated spectral analysis algorithms integrating SIM to solve the problems described above. The use of original Matlab<sup>®</sup> functions and open source internet software libraries were used to make algorithms that are able to effectively calibrate Raman spectra, classify spectra into groups and setup a foundation to facilitate referencing the calibrated data.

## **1.2 Literature Survey**

Raman spectroscopy is a technique that lends itself to fast and efficient chemical identification. Raman spectroscopy functions by utilizing a monochromatic light source to analyze materials. The monochromatic light, usually a laser, is scattered by the sample and inelastically scattered light bands are detected. The inelastic Raman bands are usually weak, which is why intense radiation sources like lasers are used. The Raman bands are associated with the vibrational modes of molecules and are shifted from the frequency of the excitation radiation. The source radiation interacts with the electron cloud of the molecules, inducing and oscillating dipoles about banding

regions. A change in the polarizability of the electron cloud in these bonding regions is required for Raman scattering to occur.

Quantum mechanically, the vibrational ground state of the molecule is excited to a virtual state. Upon relaxation, photons are emitted that correspond to both Rayleigh and Raman scattering. The Rayleigh radiation is elastically scattered and is the most intense scattered radiation. The Raman radiation consists of both Stokes and anti-Stokes bands. The red shifted Stokes bands are usually used for Raman analyses due to the higher intensity versus the anti-Stokes bands at ambient conditions. A diagram showing the excitation and relative distribution is given by Eckenrode et al. <sup>6</sup> was redrawn in Fig.1.



**Figure 1: Raman Scattering**

In the work presented here, Raman Stokes shifted bands are used for material identification. The frequency of the light source must be carefully selected because longer wavelengths may not yield intensities strong enough to yield a suitable analytical spectrum and higher frequency radiation sources may produce sample fluorescence that can interfere with the Raman spectrum.

Some key analytical advantages of Raman spectroscopy for the field, given by Eckenrode et al.<sup>6</sup>, are listed below.

- Reduced time spent on sample preparation
- Reduced interference by water, CO<sub>2</sub>, and silica
- Remote analyses with fiber optics
- Sample penetration to various depths
- Adjustable wavelength and power sources for varying sample sizes
- Equipment scale reduction potential

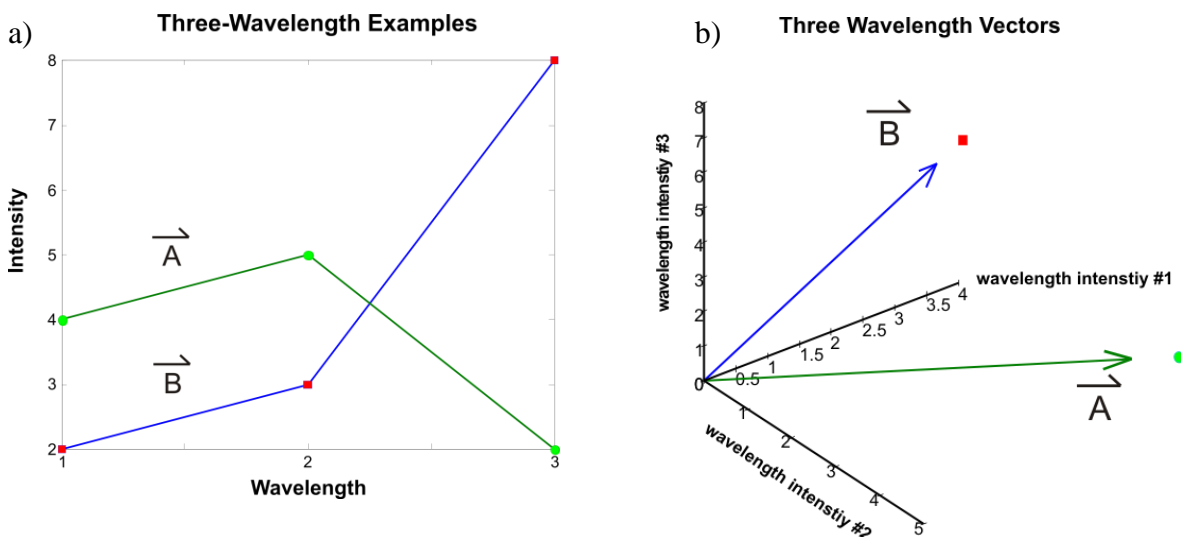
These capabilities are contributing to the growing usage of Raman spectroscopy for material identification across many scientific fields.

### **1.2.1 Spectral Identity Mapper (SIM) Theory**

SIM utilizes spectral angle mapping (SAM) and cosine correlation analysis (CCA) to differentiate samples based on the shape of their Raman spectra and to perform spectral matching of an unknown sample against library of Raman spectra. The principle use of SIM is to evaluate pixel similarities in chemical image datasets based on the shape of their corresponding spectra.<sup>1</sup>

The result of SIM for chemical imaging is chemically-based image contrast. SIM is scale invariant and can produce both qualitative identification and quantitative estimates. The qualitative identification capabilities of SIM are used here to perform wavenumber calibration and to identify Raman spectra.

The predecessor method, CCA and the first descriptions of SIM are given by Turner et al.<sup>1,7</sup> After a spectrum is acquired, detector offset and background noise are removed from the spectrum. This is achieved by acquiring a background spectrum from the system used. Comparing spectral shapes between a reference spectrum and an image dataset requires that the pixel values of the data frames, each frame corresponding to a different wavelength, be cast into multi-dimensional wavelength space so that each spectrum is represented by a single point in space where the intensity of each wavenumber is plotted on its own axis. A three-wavelength spectrum is shown below to illustrate the process.



**Figure 2: Vector Conversion of Spectra.** a) A set of three-dimensional wavelength spectra and b) the vector representation of the spectra.



The trajectory of each vector is reflective of the spectral shape. Hence, for chemically specific methods like Raman spectroscopy, the vector directions are indicative of sample composition. The tails of each vector start at the plot origin. Vectors representing similar sample compositions lie on top of one another. Samples with similar relative compositions have vectors that are parallel to each other, but with magnitudes that are representative of concentration. The angular separation between any two vectors represents dissimilarity amongst the vectors. The angle between two vectors is independent of magnitude making SIM scale invariant.<sup>1</sup>

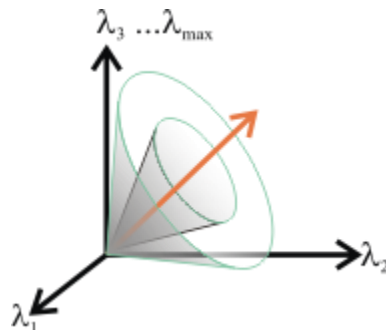
In a spectrum, the Raman bands are reflective of material composition. A material can be identified based on the similarity of its spectrum to a known set of reference spectra. However, angular symmetries could give similar results for more than one spectrum relative to a reference spectrum. While using SIM, symmetries seen in SAM and CCA are avoided by comparing results from three separate cosine correlation analyses (CCA) within SIM. This will be demonstrated in the experimental procedure. The goal with SIM is to differentiate spectra that could produce similar SAM and CCA values.

With SIM, iterative protocols of reference vectors can be avoided and the range of the chemical composition is not lost to data reduction.<sup>1</sup> SIM achieves this by asymmetrically distorting the data and assigning RGB color values to three calculated scores. The results display color contrast for the spectral image. Instead of color values, the three values can also be used to project a point in three dimensions. The three dimensional axes correspond to the three SIM scores derived from the sample. If samples are similar they will produce clusters in the three dimensions.

### 1.2.2 Cosine Correlation Analysis (CCA)

Before SIM can be utilized, a data reduction method called cosine correlation analysis (CCA) must be employed. CCA yields the statistical correlation between a spectrum and a given reference spectrum. The reference can be mathematically generated or composed of any spectrum, shape or feature. This is a very powerful aspect of SIM. It allows the flexibility of identify any spectral feature that is of interest to the analyst. The reference spectrum must contain the same number of intensity values as the spectrum or spectral feature being analyzed. Some imaging methods call the reference spectrum a “kernel”. The reference can be selected or generated in order to produce the highest potential contrast or range of correlation scores.

In order to employ CCA the data must be cast into multi-dimensional wavelength space. A desired dimensional size can be selected by drawing a point in space whose position from the origin is represented along each wavelength axis by a corresponding intensity value of the spectrum at that wavelength.<sup>1</sup> A multi-dimensional representation is given in Fig. 3. Potential data symmetries are shown by concentric cones around the reference vector (red).



**Figure 3: Multi-dimensional Vector Representation**

### 1.2.3 Spectral Data Perturbation

To perform SIM, three CCA analyses were performed. Hence, instead of a single CCA score, three CCA scores are produced in order to deal with angular symmetries. The first score is obtained from unperturbed spectra with the detector offsets removed giving the cosine angle in comparison to the reference vector. Symmetries may be found, so two mutually orthogonal perturbations are made to the raw data and CCA is performed two more times. The result is a set of three CCA scores that are highly specific to the spectral shape. A vector representation of the process is shown in Fig. 4.

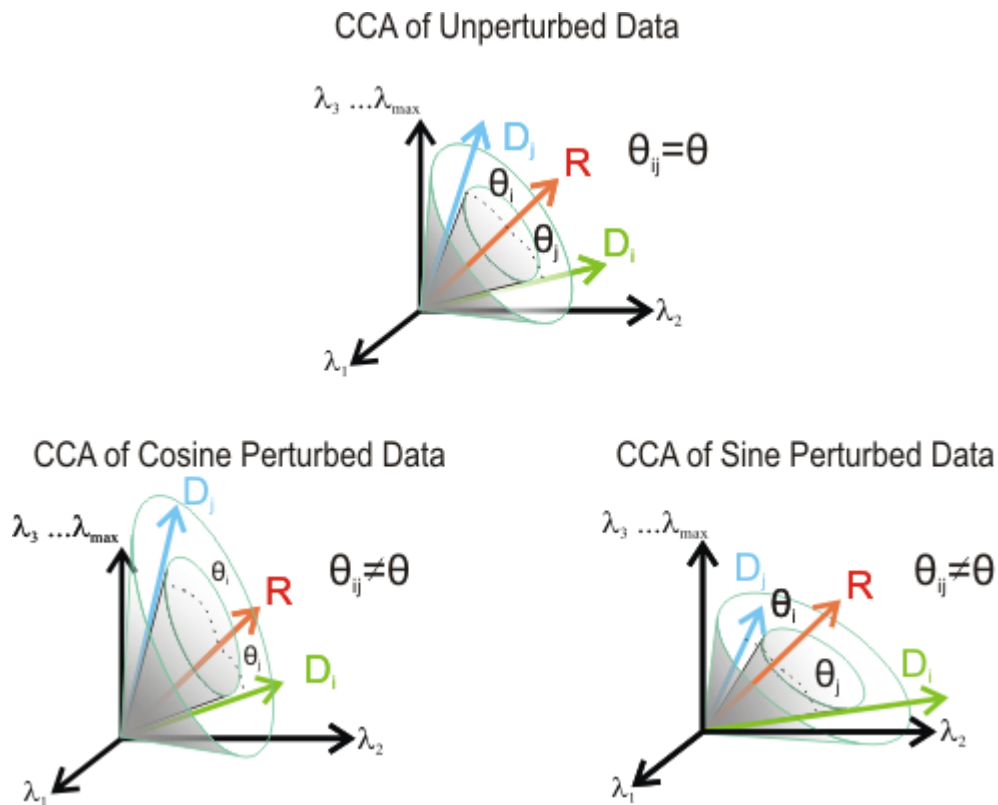


Figure 4: Unperturbed and Orthogonal Perturbations of the Data

In Fig. 4,  $R$  is the reference vector,  $D_i$  and  $D_j$  represent the two dissimilar spectra that yield the same CCA score for the unperturbed case. Hence,  $D_i$  and  $D_j$  are said to be symmetrical about  $R$ . When perturbed,  $D_i$  and  $D_j$  exhibit new angular separations relative to  $R$  and become distinguishable.

The perturbation function  $f$  and  $g$  are applied as a series of weighing functions, one for each wavelength. An example of a weighting factor application is given by Turner et al.<sup>1</sup> and is shown below:

$$f = \left[ \cos\left(\frac{1 \cdot 2\pi}{p}\right), \cos\left(\frac{2 \cdot 2\pi}{p}\right), \cos\left(\frac{3 \cdot 2\pi}{p}\right), \dots, \cos\left(\frac{p \cdot 2\pi}{p}\right) \right] \quad (1)$$

$$g = \left[ \sin\left(\frac{1 \cdot 2\pi}{p}\right), \sin\left(\frac{2 \cdot 2\pi}{p}\right), \sin\left(\frac{3 \cdot 2\pi}{p}\right), \dots, \sin\left(\frac{p \cdot 2\pi}{p}\right) \right] \quad (2)$$

In this particular case,  $f$  and  $g$  represent the sine and cosine functions, which are orthogonal functions.

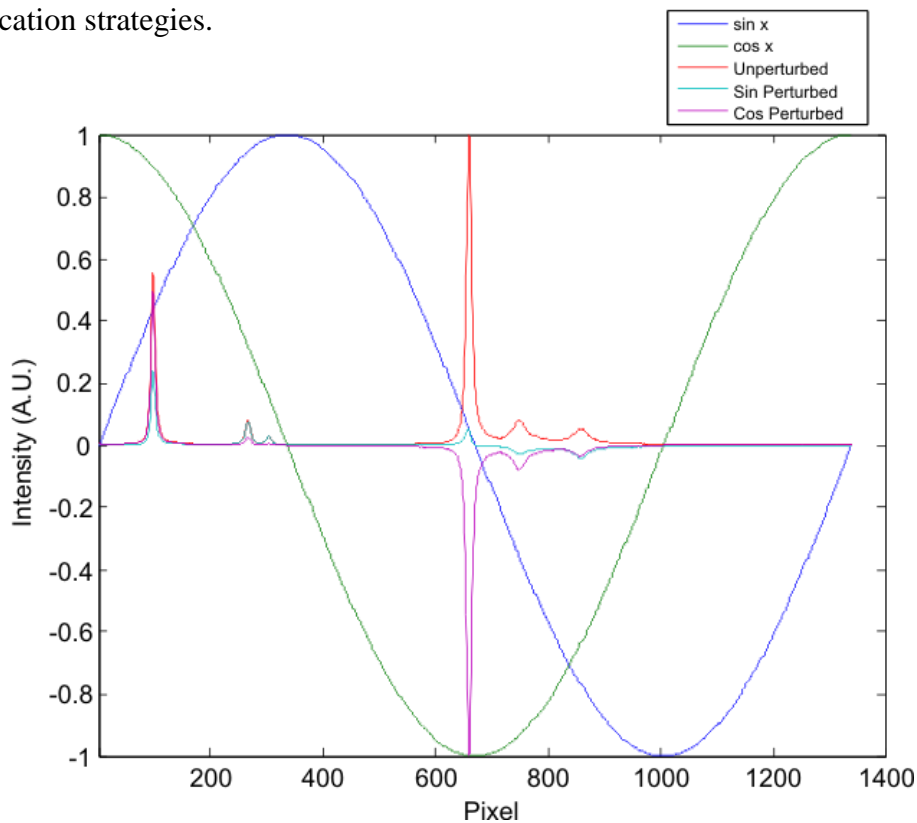
Any set of functions can be selected so as perturbation functions as long as they are orthogonal to each other. This property is represented with the equation given by Turner et al.<sup>1</sup> shown below:

$$\sum_{q=1}^p D_i^2(\lambda_q) F(\lambda_q) G(\lambda_q) = 0 \quad (3)$$

where  $q$  is the  $q$ th wavelength in the multi-dimensional space. Further details on the best choice of perturbation criteria are given by Turner et al.<sup>1</sup> These functions distort the wavelength space of the datasets so each spectral vector generates a unique set of CCA scores.

Vectors that are symmetric around a reference would normally give similar SAM and CCA scores. Different score sets are yielded when the SIM process is applied. In spectral matching applications spectra with composite scores that don't surpass a calculated or manually selected threshold scores are discounted as spectral matches.

The use of orthogonal perturbations is the SIM extension of CCA. A single period of sine and cosine functions was utilized here. Figure 5 shows spectrum and its manifestation after applying either the sine or cosine perturbations. The cosine and sine perturbation functions are shown using green and blue dotted lines, respectively. A Raman spectrum (red) is recast as a cosine perturbed (light blue) and sine perturbed (purple) set of spectra. This technique will be used in both the calibration and identification strategies.



**Figure 5: SIM Weighting of a Spectrum with Orthogonal Perturbation Vectors**

### 1.2.4 SIM/CCA implementation

Utilizing CCA, the cosine value of the angle between the spectral vector and the reference vector is used as a score for estimating how similar the two spectra are in their shape. If the reference vector and the spectral vector have the same shape, CCA will return a value of 1 because the cosine of an angle equal to 0 is 1. This indicates the spectral vector and a reference vector lie on top of each other in the multi-dimensional vector space. Spectral vectors with larger angular separation from the reference vector will yield cosine angle values closer to 0. Cosine angle is a statistically relevant and is denoted by  $r$ . While CCA results in a single  $r$  score, SIM produces three score,  $r_{D,R}$ ,  $r_{D_{cos},R}$ , and  $r_{D_{sin},R}$ . This was shown by Turner et al. <sup>1</sup> with the formulae given below, where  $D$  is a sample vector,  $D_{cos}$  and  $D_{sin}$  are the cosine and sine perturbed vectors and  $R$  is the reference vector.

$$r_{D,R} = \frac{D_i \cdot R}{|D_i| |R|} = \cos \theta \quad (4)$$

$$r_{D_{cos},R} = \frac{D_{i,cos} \cdot R_{cos}}{|D_{i,cos}| |R_{cos}|} = \cos \theta_{cos} \quad (5)$$

$$r_{D_{sin},R} = \frac{D_{i,sin} \cdot R_{sin}}{|D_{i,sin}| |R_{sin}|} = \cos \theta_{sin} \quad (6)$$

SIM is useful for a wide range of qualitative assessments. For example, SIM can be used as a matching algorithm for comparing a spectrum to a set of spectra in an image library or as a means to generate image contrast in hyperspectral image data. Another important use of SIM, introduced here, for the first time, is as a pattern recognition algorithm for identifying individual Raman bands within a spectrum. In

this last implementation, the reference spectrum is a single band or a peak-shaped segment called a kernel. The kernel is utilized as a sliding neighborhood, which is incremented across the spectrum. A SIM score is returned for each position of the kernel along the length of the spectrum. Alternatively, a CCA score could be calculated if data symmetries are not problematic. This type of sliding kernel SIM or CCA analysis is useful to identify features within a spectrum for application like automated band calibration.

As part of the work described here, an automated calibration algorithm was developed based on the sliding kernel CCA procedure. CCA was performed as a sliding frame (kernel) with a 9-pixel spectrum taken from the center of a Lorentzian shaped reference vector to identify Raman bands in the spectrum of a calibration standard. The sliding frame was iterated across a sample spectrum after replacement of the sample spectrum peaks with Lorentzian shape bands to remove baseline non-uniformities. SIM generated triplet score sets for each frame shift across the spectrum. The scores were used to identify Raman bands within the spectrum so that it could be compared to the known position of the standard sample.

### **1.2.5 Spectral Analysis Scope**

Assessing and comparing other chemical analysis methods available can be difficult. Modern methods utilize an amalgamation of scientific methodologies to provide spectral analysis of Raman spectra. This can make it difficult to provide a direct comparison of analysis methods because there are many ways in which the methods are combined.

Although there are many resources, a central one is lacking. This may be because methods are continuously evolving. Some chemical analysis methods and commonly used signal processing techniques are given here for comparison with SIM. Many extensions of these methods exist, however.

A category of chemical analysis methods called “chemometrics” rely on the use of computational methods in order to gain information about chemical systems. SIM can be considered a chemometric method. These methods are generally multivariate. They also have very strict procedures that must be adhered to in order to function properly for a given analysis.

Chemometric methods provide descriptive and predictive information about chemicals utilizing data driven computer methodologies. The data obtained is used to develop descriptive and predictive math models based on the components of the chemical systems being analyzed. Model development often involves various mathematical and statistical regression techniques that can involve multiple parameters.

Some chemometric methods are also considered “data reduction” techniques because the data is reduced to a smaller set of variables. The techniques that will be surveyed are hyperspectral imaging with spectral mixture analysis (SMA), spectral unmixing, spectral end member analysis, principle component analysis (PCA), factor analysis (FA), cluster analysis (CA) and multi-variate curve resolution (MCR). Other notable methods are partial least squares (PLS), artificial neural networks (ANN) and detrended fluctuation analysis (DFA).

All of these methods can be invoked for processing and determining various forms of information for multispectral and hyperspectral imaging. This information includes classification of spectra and correlation to a reference spectrum.



In order to produce the best information from a chosen chemometric method, an analyst should implement signal and data processing techniques. Once a basic understanding of the chemometric methods and the techniques they utilize is established, a fair comparison of the analytical methods can be performed.

Chemical analysis methods can utilize “data mining”. Modern data mining involves the use of computational methods in order to extract meaningful information from datasets. Most modern chemical analytical methods use computational data mining methods to extract datasets from raw instrumental data. Data pre-processing may be required depending on the data selected for analysis.

A primary understanding of chemical signals and their measurement is central to all analysis methods. A fundamental review of instrumentation and signal acquisition is given by Skoog et al.<sup>8</sup> Spectroscopic based chemical signals must be extracted from the chemical systems that are being studied. A stimulus is applied to the chemical system and the response monitored. Modern spectroscopic measurements follow this protocol exploiting various physical properties of the chemical system being analyzed.

The exploited physical properties contain information about the chemical system. This information can be categorized physically within data domains. The instrumentation extracts chemical information encoded in chemical systems and it translates the information into alternative data domains by utilizing electrical domain signals. Electrical domain signals can be converted to digital data domain signals, which are used to transmit and manipulate data more efficiently.

Most spectroscopic instrument detectors produce electrical domain signals for photonic events over a user defined time period. The detector output is recorded and can be manipulated by software to provide a meaningful response.

It should be understood that every component in the instrument can affect signal measurement characteristics such as accuracy, precision, sensitivity, detection limit, dynamic range, selectivity and bandwidths of operation. Details of how these criteria affect chemical signals are given by Skoog et al.<sup>8</sup>

It is important to understand that every analytical measurement is actually composed of the analytical signal and noise. Noise can come from multiple sources and can interfere with all measurement characteristics. It can be considered as a type of random error. The smaller the signal, the greater effect noise has on the overall analysis. This is why the signal to noise ratio (S/N) is used to describe the quality of instrument measurements. A signal to noise ratio  $\leq 2$  generally means the signal is indistinguishable from the noise. It is customary to try to obtain the largest analytical signal intensity possible in order to improve the signal to noise ratio. An analyst should also be aware of systematic error.

There are many hardware and software methods for extracting a signal from noise and some will be given in the next section. In general, the signal to noise ratio can be improved by increasing the number of measurements taken. This is because the signal to noise ratio is mathematically proportional to the square root of the number of measurements. The proportionality of the signal to noise is seen in the formula below,

$$\frac{S}{N} = \sqrt{n} \frac{S_x}{\sqrt{\sum_{i=1}^n (S_x - S_i)^2}} \quad (7)$$

where  $n$  is the number of spectra,  $S_x$  is the sample mean and  $S_i$  is the  $i$ th measurement.<sup>8</sup>

### 1.2.6 Spectral Signal Processing

There are many signal processing techniques to compare with SIM. Some of the techniques below are used within SIM. Care should be taken when using signal processing techniques. These techniques can have many disadvantages including the introduction of noise, signal distortion, bandwidth limitation and computational inefficiencies. Generally, a combination of signal processing methods is used to provide the best analytical results.

The main advantage of signal processing techniques is the ability to extract meaningful chemical signals and optimize physical measuring techniques. Other advantages are given by Professor Tom O'Haver.<sup>9</sup>

Signal processing techniques generally require the use of computers for the mathematics used because of the sizes of the image data sets involved. The simplest of all the techniques demonstrated by O'Haver is the usage of spectrum arithmetic.<sup>9</sup> These include spectrum addition, subtraction, multiplication and division.

Spectrum addition techniques are used for smoothing and obtaining the statistical advantage of increased spectral acquisitions. Problems can arise if data in the spectrum is from interfering sources. Background subtraction directly removes contributions to a signal that are not from the chemical analyte. Subtraction alone can present problems if the background acquisition conditions do not match those of the sample and if the background spectrum is not carefully obtained.

Spectrum multiplication is generally used to apply spectral filters and for test various physical and theoretical interferences on spectral signals. Spectrum division between two spectra provides a ratio spectrum. If the ratio is constant over some range,

the spectral shapes are considered the same over the selected region even though the intensities may be significantly different; a scale invariant shape technique.

The above techniques are usually not sufficient alone for complex spectral analysis. Advanced spectral analytical techniques are normally required. However, most advanced techniques usually just implement some sort of spectral arithmetic in a specific procedure. Some of these techniques are given by O'Haver.<sup>9</sup> It is usually more important to understand the information about the data being processed.

Calculation of the noise observed in a stimulated chemical system is necessary in order to remove its effects on the analyte signal. Possible types of noise are given by Skoog and O'Haver.<sup>8-9</sup> O'Haver gives some noise estimation techniques in his examples. O'Haver also covers the basis of different types of noise as well as filtering and smoothing techniques. The smoothing and filtering of samples must be done carefully in order to prevent distorting the true signal. The original sample data should be maintained for referencing and reprocessing. It should be understood that smoothing/filtering the data causes the data to be reduced and the original data points are lost in the processes.

Three smoothing techniques that can reduce noise are rectangular, triangular and Savtisky-Golay methods.<sup>9</sup> It is important that the independent variable spacing for a spectrum is uniform to prevent the introduction of new distortions. Savtisky-Golay smoothing is used to decrease signal distortion, while reducing noise with least squares fitting of the data.

Implementing smoothing techniques can lead to data loss in the form of edge effects and averaging.<sup>9</sup> Signal amplitude can be lost if the ratio of the smooth width to

the width of the peak is not taken in to account. Increasing the number of data points or reducing the interval at which the data is taken can help reduce smoothing distortions.

Smoothing techniques can present problems with quantification of samples if smoothing is not applied to all the samples involved. Any standards should be smoothed in a procedure similar to sample data. Smoothing challenges can also be encountered if there are random spikes in the spectrum or if the data is oversampled. O'Haver covers these scenarios in some detail.<sup>9</sup> Smoothing can be considered a pre-processing technique.

Peak identification can be achieved with differentiation of spectral data. Problems can arise with differentiation if the intervals between spectral data points are not consistent. With differentiation, a peak can be identified by taking its first derivative and observing where the zero crossing takes place in the resulting plot. "A problem with differentiation is that it degrades the signal-to-noise ratio, unless the differentiation algorithm includes smoothing that is carefully optimized for each application".<sup>9</sup>

Another problem is false zero crossing after differentiation. O'Haver offers some smoothing and interpolation solutions to these problems. Derivative methods are linear and can have problems with non-linear spectra because the derivative is proportional to the original signal and this should be understood for quantization.<sup>9</sup> Trace level signal analysis with differentiation is possible, but the user must be aware of the proper smoothing processes to utilize differentiation techniques correctly.

Obtaining better peak resolution (sharpening) helps to identify chemical components in samples by making their signal intensities identifiable. O'Haver presents a commonly used peak resolution algorithm, deconvolution techniques and guidelines

for implementing them. A disadvantage is that these processes can also decrease the signal to noise ratio if not implemented properly.

Convolution is used for simulating optical effects on data, filtering spectra and implementing analytical test procedures.<sup>9</sup> O'Haver gives some filtering methods that can be applied. Filtering methods generally take advantage of Fourier mathematics or system modeling. Careful selection of convolution parameters, specific to sample spectra, must be performed in order to obtain meaningful results.

With deconvolution broadband functions, each potentially overlapping signal has to be known before they can be removed. The overlap can be removed in the Fourier domain. O'Haver reviews the application of Fourier mathematics to spectra.<sup>9</sup> O'Haver acknowledges deconvolution as an artificial procedure to reverse distortion. Deconvolution can also cause signal to noise degradation. An interesting note is that Fourier techniques can be applied in real-time to live signals with the use of signal processing chips.

### **1.2.7 Spectral Analysis Methods**

Many methods exist for producing predictive models for sample composition and quantification of sample components. SIM has the potential for sample decomposition.<sup>1,8</sup> For elemental concentration in mixtures linear regression techniques are typically used. Linear regression models can be based on peak intensities or peak areas. If there is peak convolution, integration techniques require a known peak shape and a fitting technique to determine true peak areas and intensities. Inverse least squares techniques can be used when the concentration of the components is not known in a mixture.

Multi-component spectroscopic techniques are usually based on least squares methods, but require some idea of the known components. An inverse matrix to find sample components can only be solved for with square matrices.<sup>9</sup> Analysts must account for background intensities, noise, wavelength dependent noise and element weighting factors. Implementing a multi-component technique usually requires training datasets.

Transforms must usually be applied to non-linear systems in order to convert them to linear models so that solutions to unknown component mixtures can be generated. Noise can be introduced in the conversion. Iterative methods are generally applied to non-linear systems. All non-linear parameters must be known for assumptions/models to be validated. Fitting error calculations must be performed for the quality of the fit to derived models. O'Haver gives some non-linear methods, requirements and example procedures for this approach as well as possible modeling errors.

Hyperspectral imaging is a technique for chemical identification of individual chemical components in an image by extracting data, on a pixel basis, from a continuous band of spectral wavelengths.<sup>10</sup> As previously explained, SIM is a useful method for creating chemical-based image contrast in hyperspectral imaging.

Spectral vectors extracted from hyperspectral images will form clusters of spectral data that are specific to the chemical species. Some important properties of hyperspectral imaging are spatial resolution, spectral mixing, spectral reflectance, spectral radiance and source illumination interferences.<sup>10</sup>

Understanding spectral mixing gives the basis for spectral unmixing. Spectral unmixing is used to determine the components in a sample mixture. Spectral unmixing

provides “endmember spectra”, which are the pure component in a mixed spectral image. End members spectra can be extracted by spectral mixing and unmixing techniques. An interesting application of this is partial unmixing of a spectral image.<sup>10</sup> Spectral unmixing is performed with the use of “matched” filters. Closely evolved techniques for determining the components in hyperspectral images are spectral mixing analysis and end member spectra analysis.

Principal component analysis (PCA) is a statistical technique for finding patterns within data sets. It is a widely utilized tool for prediction, data compression and object identification. An elementary review of PCA is given by Lindsay Smith’s, “A tutorial on principal component analysis”.<sup>11</sup> Many scientific fields utilize PCA including computer science for facial recognition, biology for many methods of cell analysis, and material engineering.<sup>12-14</sup>

PCA can analyze multi-dimensional data making it a useful tool for multi-dimensional and hyperspectral data analysis. PCA is a data reduction method. PCA does not try to search for supporting factors in observed spectra it only shows relationships between observed measurable data variables.

Factor Analysis (FA) is a data reduction method, but the goal of FA is to find the underlying factors responsible for observed spectra. Factor analysis and PCA developed from statistical psychometric analysis.<sup>15</sup> Factor analysis can be more difficult to implement than PCA because models are based on theoretical assumptions that must be carefully modeled and tested. Two reviews of FA are Jamie DeCoster’s, “Overview of Factor Analysis”<sup>16</sup> and Daniel Denis, “Factor Analysis”.<sup>17</sup> Denis describes FA as a method for reducing the dimensionality of data.



There are two main types of factor analysis including exploratory factor analysis (EFA) and confirmatory factor analysis (CFA). They are based on the common factor model. A description of the common factor model is given by DeCoster.<sup>16</sup> In addition to the number of factors, the degree to which they influence the observed variable is estimated. Individually, each factor is assumed to contribute to the data variance. Factor scores can be generated to obtain each factor's influence in the observed data. DeCoster gives some guidelines for implementing FA.

Factor analysis has been extended into many scientific fields to help solve many problems like cancer imaging<sup>18</sup> and has been attempted to be automated for other scientific tasks. An interesting extension of factor analysis is parallel factor analysis (PARAFAC). It is also known as “canonical decomposition”. FA methods must be strictly followed for proper data reduction and assignment of significance contributions to derived factors.

Cluster analysis is a data mining method for identifying groups within data sets based on variable observations. The goal is achieved by recognizing distinct groups based on the spatial relationship of the observations.<sup>19</sup> Cluster analysis has been applied widely in imaging spectroscopy and biological analysis.<sup>20, 21</sup>

Peter Tyrfos offers some technical implementations of cluster analysis.<sup>20</sup> Tyrfos explains that for a large number of variables cluster analyses can be difficult to visualize and he offers some techniques for distinguishing clusters. One of the techniques is the use of Euclidean distancing. The general distance equation is given by,

$$D(i, j) = \sqrt{\sum_{i=1}^n (i_i - j_i)^2} \quad (8)$$

where  $D$  is defined as the distance between points  $i$  and  $j$  in a Cartesian system. This can be extended to multiple dimensions and normalization methods are suggested to make the math simpler.

Using Euclidean distance alone and considering each observation as an individual cluster, mergers can be formed amongst the individual clusters. The data with the smallest distances between one another are grouped until distinct clusters are formed. These new clusters can be observed with a dendrogram illustrating the data clusters. Tyrfos calls this the “nearest neighbor method”.

Other methods are given, like furthest neighbor and average neighbor methods, but they require a careful understanding and observation of the data in order prevent inaccurate data clustering. These are considered hierarchal agglomerative cluster methods. There are also hierarchal divisive and non-hierarchical methods. Cluster analyses can also be extended beyond observational data to group variables, which may require the inclusion of weighting coefficients. There have been some attempts to automate cluster analysis.<sup>22,23</sup>

Artificial neural networks (ANN) are a type of computer learning technique. A simple introduction about how neural networks function is given by Carlos Gershenson.<sup>24</sup> Neural networks have found wide spread use in the imaging and scientific community.<sup>25-27</sup> One interesting application is the use of fractal ANN's.<sup>28</sup>

Three prominent methods for determining the spectral components in a sample mixture are partial least square regression (PLS), multivariate curve resolution (MVR) and spectral unmixing. The goal of partial least squares regression (PLS) is similar to factor analysis in that the goal is to try to determine the underlying dependent variables

that lead to an observable using predictors instead of factors. A review of PLS is given by Hervé Abdi and Michael Haenlein.<sup>29,30</sup>

Multi-variate curve resolution is another decomposition technique that is widely used to identify components that contribute to an observed spectrum. A review of the technique can be found in chemometric texts.<sup>31</sup> MCR is used in conjunction other correlation techniques. Spectral unmixing has been previously introduced.<sup>11,32</sup>

Detrended fluctuation analysis (DFA) is a method for observing relations amongst time varying data. Some complex applications of DFA exist for analyzing images from all areas of science.<sup>33-35</sup>

### **1.2.8 Summation of Advantages and Disadvantages**

A summary of some the advantages and disadvantage for some spectral analysis methods are given below. The use of data reduction provides the ability to describe data using descriptors such as data variance. Positive covariance can indicate relationship amongst data variables as described in the PCA and FA literature.

Multivariate techniques offer some graphical representation of higher dimensional data. Scoring methods can be used to show significant relationship amongst data. Within relational information about the composition, data reproduction and mapping makes it possible to simulate experiments and organize data. Unknowns without *a priori* information can also be characterized. These features make chemometric methods powerful analysis tools.

After reviewing the literature for signal processing techniques and analysis methods, the most prominent disadvantages would be the lack of an “automated” spectral analytical method to large datasets. Another disadvantage is the introduction

of noise into a spectrum during signal processing. Some of the methods also require cross checking data and extensive iterations to properly fit data models.

Implementing the techniques properly requires highly trained analyst in multiple fields to interface all the different scientific disciplines used. The SIM method developed here is designed to present the user with some immunity from the above problems.

SIM provides the ability automate data classification and calibration of large data sets without extensive training of the underlying methods. SIM, when used with Lorentzian band replacements, avoids the potential signal to noise problems seen with peak differentiation described previously. This leads to better visualization and matching of spectral data. SIM is also able well suited to rendering its results using RGB (red, green, blue) color mapping or three-dimensional cluster plots, an natural extension of its three member score set. SIM can utilize spectral vector magnitudes to quantify the composition of samples avoiding integration methods which can require delicate smoothing procedures, as well as possible introduction of noise and data distortion.<sup>9</sup>

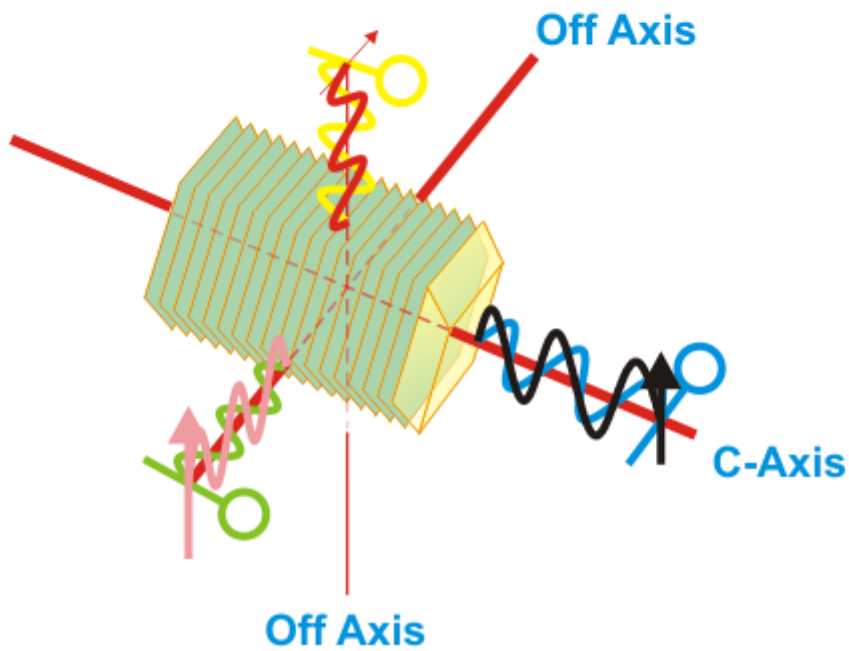
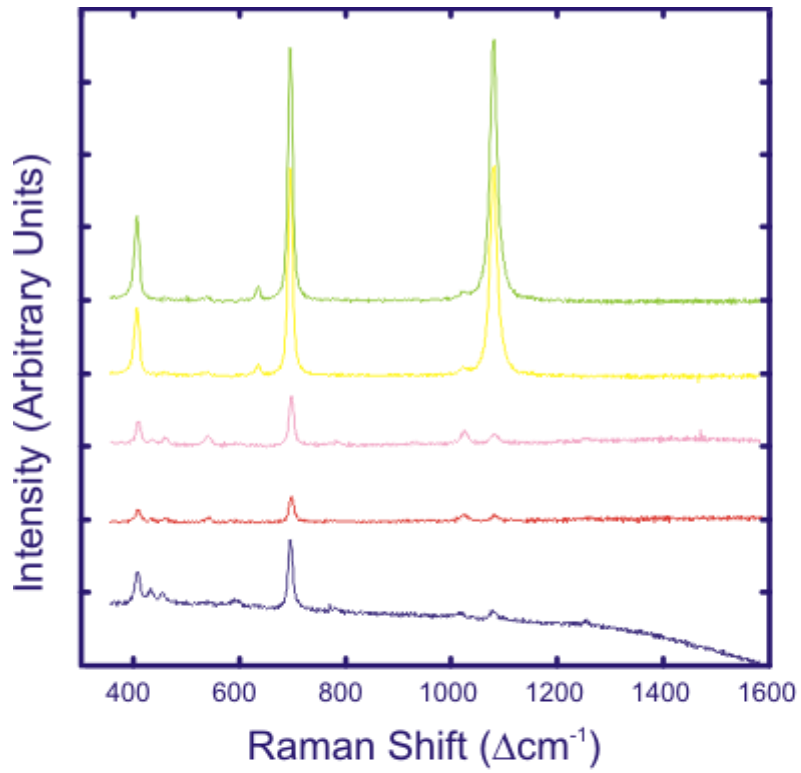
## **CHAPTER II**

### **EXPERIMENTAL**

#### **2.1 Samples and Apparatus Configuration**

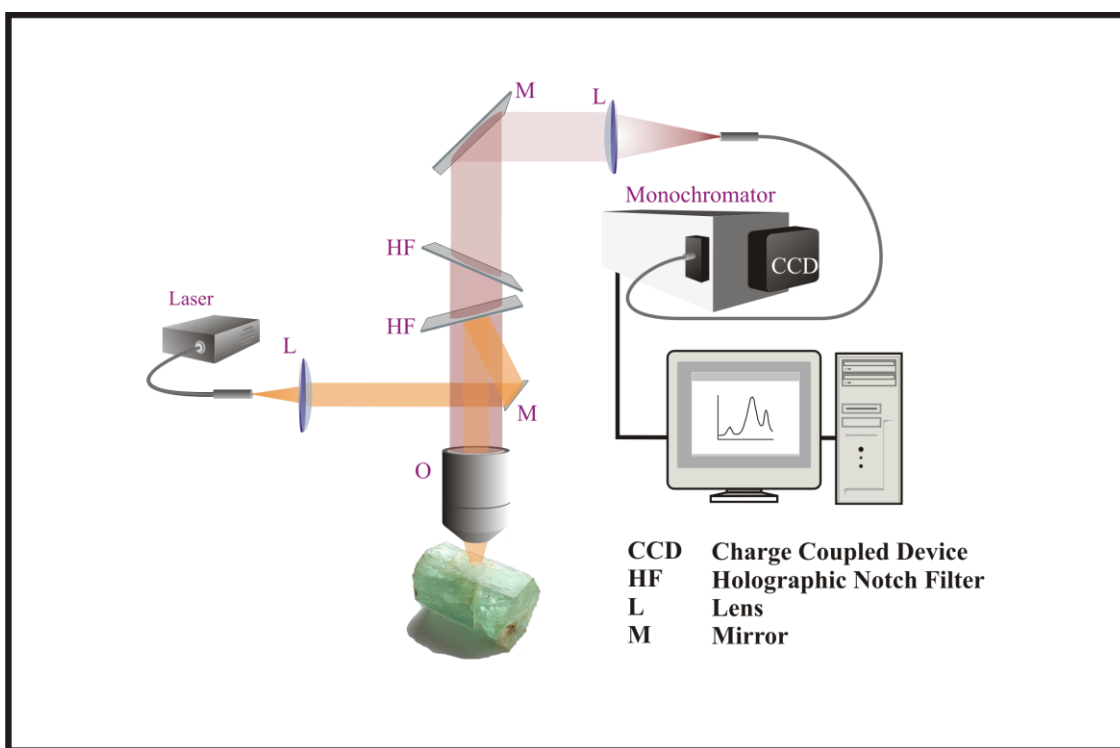
In order to develop the Raman spectral database, a wide range of samples were collected. The samples consisted mostly of minerals and some biological materials. Spectra from several orientations of the samples were acquired. This was done in order to account for the anisotropic behavior of the materials.

Polarization dependent differences are also observable when using plane polarized excitation sources. Figure 6 shows how polarization effects can influence spectral intensities. The use of circularly polarized light sources can help mitigate the effects of polarization due to sample orientation.



**Figure 6: The Effect of Laser Polarization State and Crystal Orientation on the Raman Spectrum**

Sample data was collected by several different analysts and instrument configurations. The primary configuration used while collecting data involved two lasers sources, a 1W 785nm red laser and a 1W 532nm green laser. The laser light path included a collimating lens, mirror, holographic rejection filters, focusing objectives, sample, focusing lens, fiber optic cable, monochromator and CCD detector. The collected data files were operated on by a MATLAB<sup>®</sup> coded version of SIM. Figure 7 shows a description of the Raman instrument configuration.



**Figure 7: Raman Instrument Configuration**

## 2.2 Sample Testing

While testing the samples, care had to be taken while handling the materials. Some samples were so fragile that care was needed to prevent samples from breaking apart or contaminating the optics. Some of the samples were odd shaped and needed support in order to orient the samples properly. The intensity of laser also presented

challenges. The main laser used was a 786nm at <1W power to prevent burning and sample fluorescence. If the 785nm appeared to burn the material, the 532nm laser was used to acquire the sample spectrum.



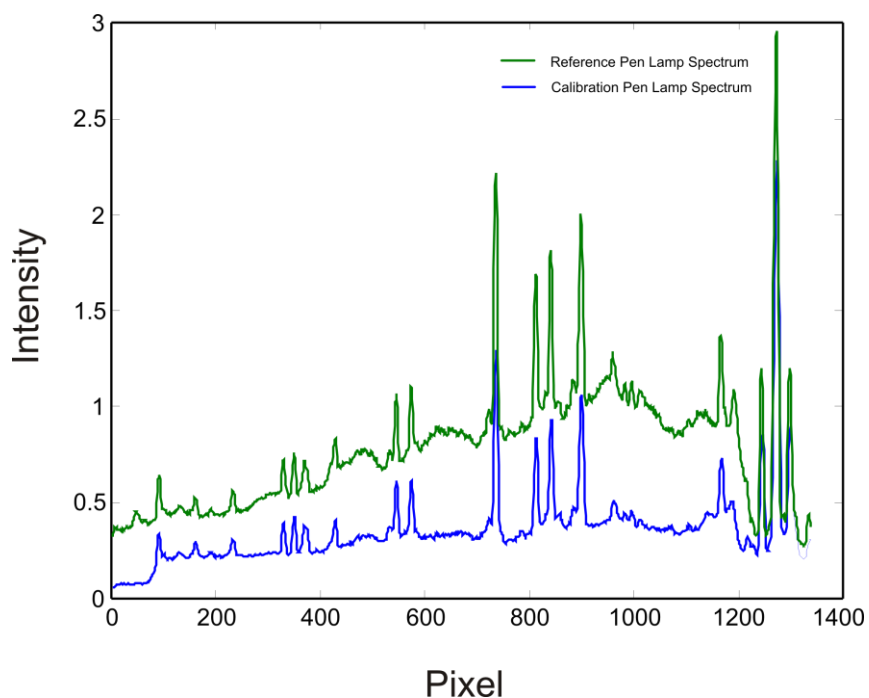
## **CHAPTER III**

### **SIM CALIBRATION**

#### **3.1 SIM Pen Lamp Calibration**

Knowing the wavelengths of all the Raman bands in a standard and observing the Raman shift values of the standard on each use of the spectrometer enables correction factors to be obtained and applied to the sample data. This strategy was used by SIM to properly calibrate the sample peaks. The calibrated data is utilized for identification and analysis of spectra. If this method is adopted by others, wavelength corrected data can make the identification of unknowns easier.

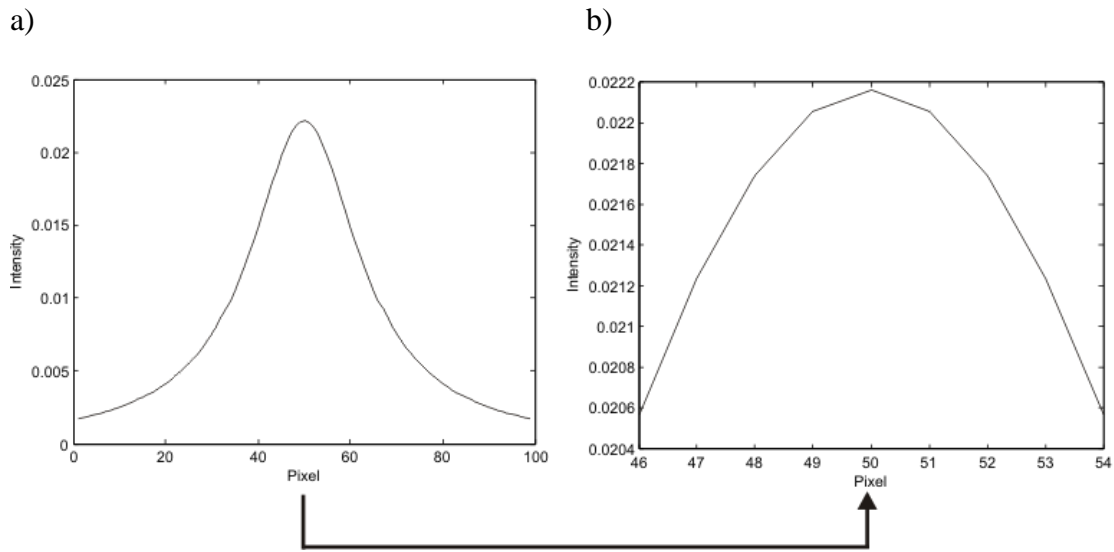
In order to calibrate the Raman spectra, a spectrum from a calibration standard is needed to account for potential differences in instrumentation and other acquisition parameters. The calibration standards used here were neon & xenon penlamps. Examples of a xenon penlamp reference spectrum and a calibration xenon penlamp spectrum (taken each time spectra are acquired) are shown in Fig.8.



**Figure 8: Xenon Pen Lamp Reference Spectrum and Calibration Spectrum**

The emission lines from the pen lamps can be referenced to known emission lines within data sources such as the Handbook of Chemistry and Physics. Knowing these emission lines, a calibration penlamp spectrum can be collected and referenced every time data is collected. Peak positions in the calibration spectrum can be shift-corrected based on the known emissions in the reference spectrum.

In order to locate the specific Raman bands required to calculate the pixel to shift, a method to identify the calibration spectrum peaks is needed. SIM was used for peak identification by comparing a Lorentzian shaped reference vector kernel to the calibration spectrum, wavelength by wavelength, starting at the beginning of the pen spectra then working through the end in a sliding neighborhood fashion as described earlier. The Lorentzian kernel is shown in Fig.9.



**Figure 9: Lorentzian Reference Vector** a) Full Lorentzian Band

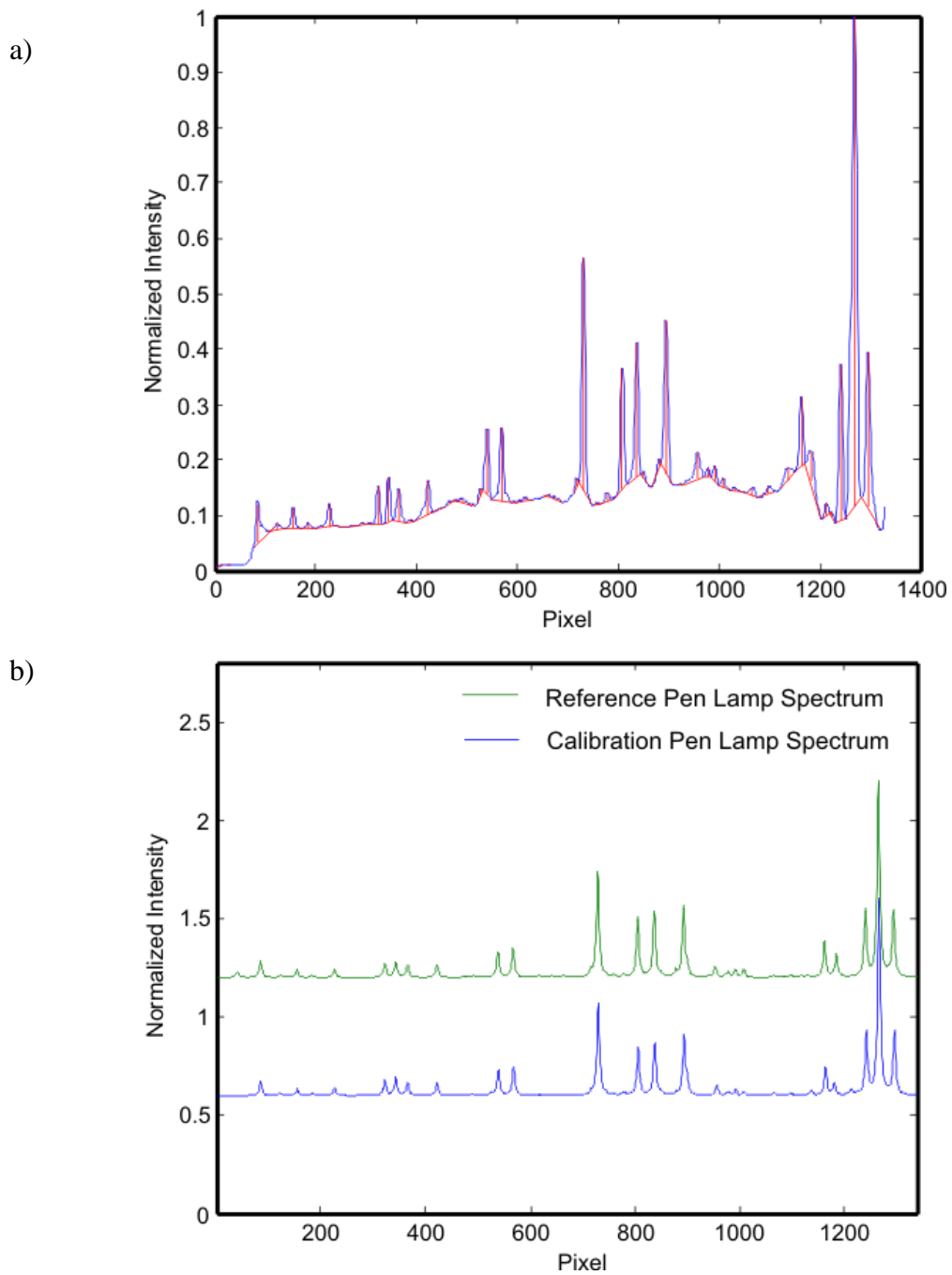
b) Lorentzian Band Kernel.

The pixel size (number of wavelengths) of the vector used can be selected as a user preference. The mechanism for comparing the Lorentzian vector to the calibration spectrum is independent of the user selected size of the Lorentzian reference spectrum. A 9-pixel Lorentzian shaped vector from the peak/center of a Lorentzian band is used here. The Lorentzian vector is compared to a 9-pixel section of the calibration pen spectrum starting at the beginning of the penlamp spectrum and is iterated across the spectrum until it reaches the end of the pixels. The sampled pixel region qualifies as a peak if its SIM scores meet a calculated or established threshold value. The threshold value is near one, but can be lowered to account for noise-based deviations from the kernel. A composite SIM score, calculated as the product of the three CCA scores, is compared to the threshold value. It should be noted that the reference vector is

perturbed by the same perturbation function as the data spectrum when performing this procedure.

### **3.2 SIM Spectral Matching**

In order to generate the SIM correlation scores the spectra are normalized in order to make the SIM algorithm computationally simpler. When a correlation is found between the Lorentzian shaped vector and a frame in the calibration spectrum a peak marker is positioned at the identified peak position. Baselines for the identified peaks are established and peak intensities are determined. The identified bands can be replaced with Lorentzian bands of similar amplitudes to the Raman bands producing a Lorentzian replacement of the data. The Lorentzian band replacements for the reference and calibration spectra are shown in Fig. 10.

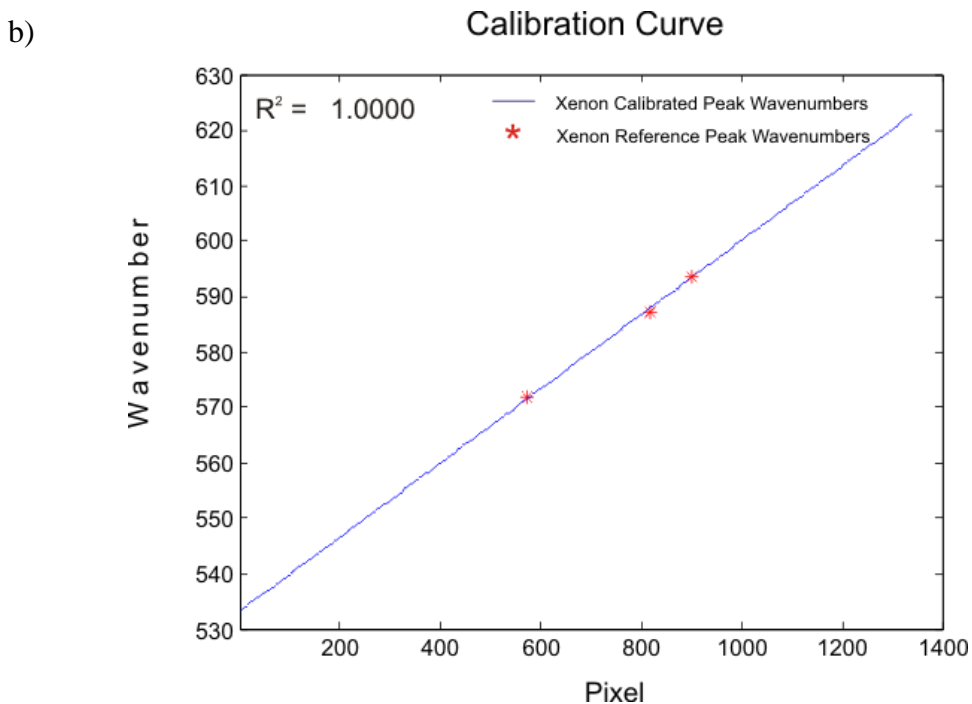


**Figure 10: Generating Lorentzian Replacement Spectra** a) Peaks identified in the reference pen lamp spectrum with drawn baselines and b) Lorentzian band replacements for the reference spectrum and calibration spectrum.

In the work presented here, the five most intense bands in the spectra are used for the shift calibration. A first order polynomial calibration curve fit indicates how well the average pixel wavenumber shifting procedure worked. The average shift is then applied to the sample spectra. The five peaks used for a shifting and a calibration curve are shown in Fig. 11.

a)

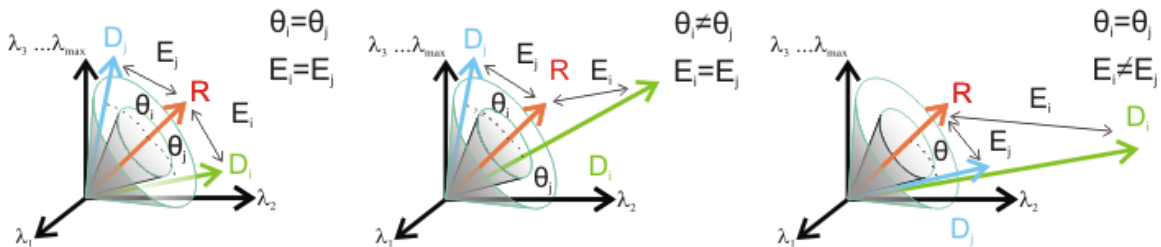
Xenon Reference Pen Lamp Spectrum		Xenon Calibration Pen Lamp Spectrum	
Normalized Intensity	Pixel	Normalized Intensity	Pixel
1.0e+003 *		1.0e+003 *	
0.0009	1267	0.0010	1266
0.0004	731	0.0005	730
0.0003	895	0.0003	894
0.0003	1242	0.0003	1240
0.0002	837	0.0003	836



**Figure 11: Pixel Shifting and Calibration** a) The five peaks used to calculate peak shifting and b) a calibration curve fitting the shifted xenon reference peak intensities.

After a calibration curve was fitted for these bands an R-squared near 1 value was calculated. Euclidean distance between the calibrated peaks and the reference peaks was calculated close to 0. Euclidean distance is used here as an algorithm operating parameter that indicates how well the calibration procedure performed. Euclidean distance values closer to 0 indicate a more robust calibration.

Euclidean distance measurements can also be used to compare vectors to a reference as an alternative to SIM. Any two data points in n-dimensional Euclidean space that lie an equal distance from a third point will yield the same Euclidean distance and can be assigned as equally likely matches to the reference. A demonstration of vectors equidistant to a third vector and one with similar angular distance are shown in Fig.12.



**Figure 12: Similar CCA and Euclidean Distance Values Can Result Due to Angular Symmetry and Similar Vector Lengths**

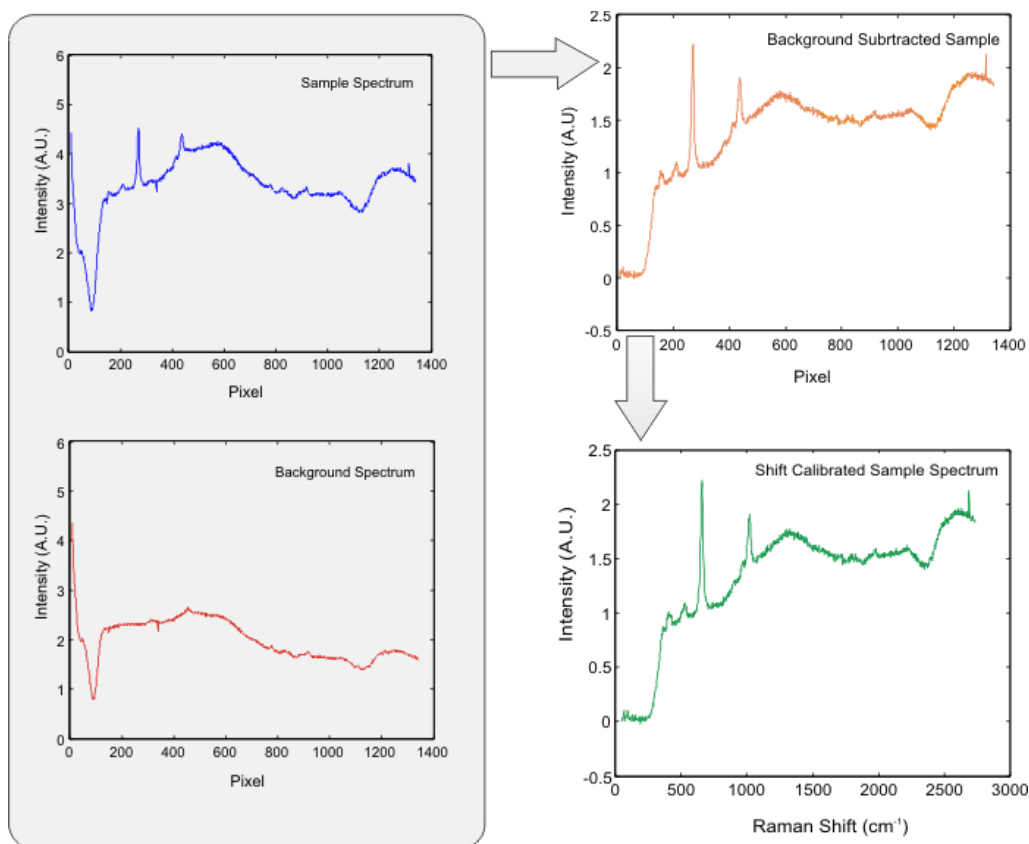
The potential for unwanted symmetry about a hypothetical cone around the reference vector is the primary reason to utilize SIM. SIM is also scale invariant making it useful in the case of scale varying data. Euclidean distancing can fail in the three cases shown in Fig. 12, where E is the Euclidean distance and  $\theta$  is the angle between sample vectors. Mahalanobis distance measurements are also useful for analyzing data with varying scales. The Mahalanobis distance between a point and the

center of a data class to which it might belong is divided by the width of the data class along the direction joining the two points.<sup>1</sup>

A comparison of SIM and distancing methods will be given in the results section. Without SIM, the possibility of falsely assigning two dissimilar spectral vectors as being similar to each other remains and is a central problem for CCA, SAM and Euclidean distancing methods.

### 3.3 Applying Calibrations to Spectra

Applying a calibration to the sample spectra is straightforward once the number of shift pixels is determined. First, the sample spectra are background subtracted and then the pixel shift is applied. The pixel is representative of a spectral wavenumber shift. The spectrum calibration procedure is shown in Fig. 13.



**Figure 13: Background Subtracted and Raman Shift Calibrated Spectra**



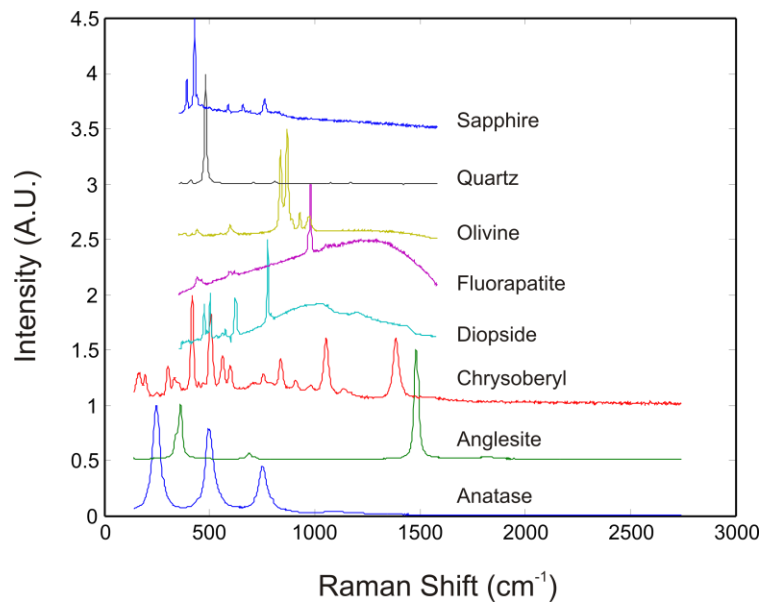
## CHAPTER IV

### SIM SPECTRAL IDENTIFICATION

#### 4.1 Spectrum Identification with SIM

The procedure for identifying spectra using SIM can be manually configured to obtain the best performance for a given data set. One protocol will be given below.

Spectra from the set of mineral species used to demonstrate SIM are shown in Fig. 14.

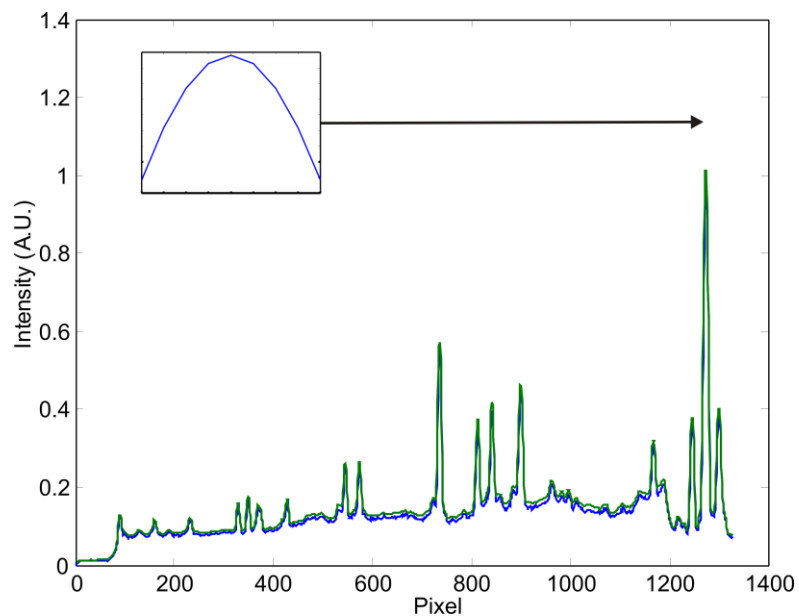


**Figure 14: Dataset of the Minerals Used for the Mineral Identification Protocol**

The data must first be cast into a common spectral range in order to prevent SIM errors due to different sampling ranges and sampling rates. The peaks in a spectrum are identified using a procedure similar to the xenon pen lamp calibration procedure in chapter 3. The sample spectrum is recast with Lorentzian peaks to remove baseline artifacts.

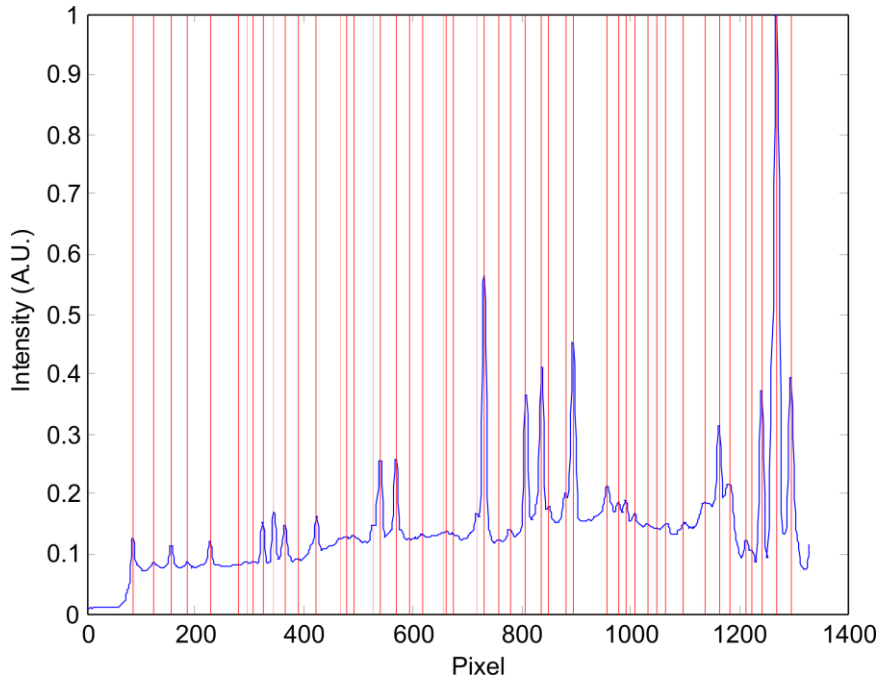
In this procedure, a Lorentzian band shape is selected as a reference kernel to help identify the spectral features of interest. The reference kernel can be any shape or feature of interest to the analyst (i.e. shoulder peaks), however. The width of the selected kernel has to be an odd number of pixels. For peak identification, Lorentzian, Gaussian or Voigt can be used.

Parameters such as the full-width half max (FWHM) can be selected as a user preference. A SIM threshold is calculated or selected in order to control the accuracy rate in identifying true peaks. Figure 15 shows a Lorentzian band (kernel) used to slide through a sample spectrum.



**Figure 15: The Lorentzian Band Reference Vector is used as a Sliding Window (kernel).**

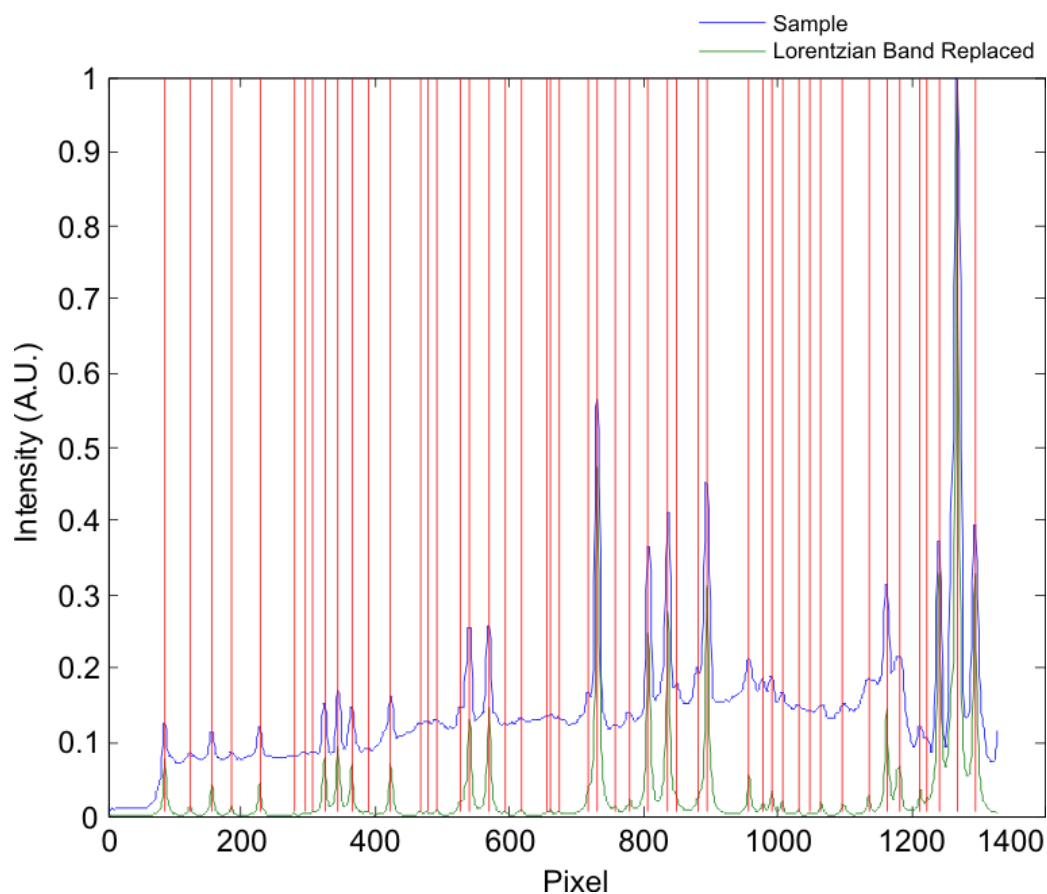
In Fig.15, the raw data (blue) is first smoothed using a median filter. The output is the smoothed (green) spectrum. All of the possible peaks that were identified in the smoothed spectrum are marked with vertical lines. Peak markers are shown in Fig. 16.



**Figure 16: SIM-based Peak Identification within the Spectrum.**

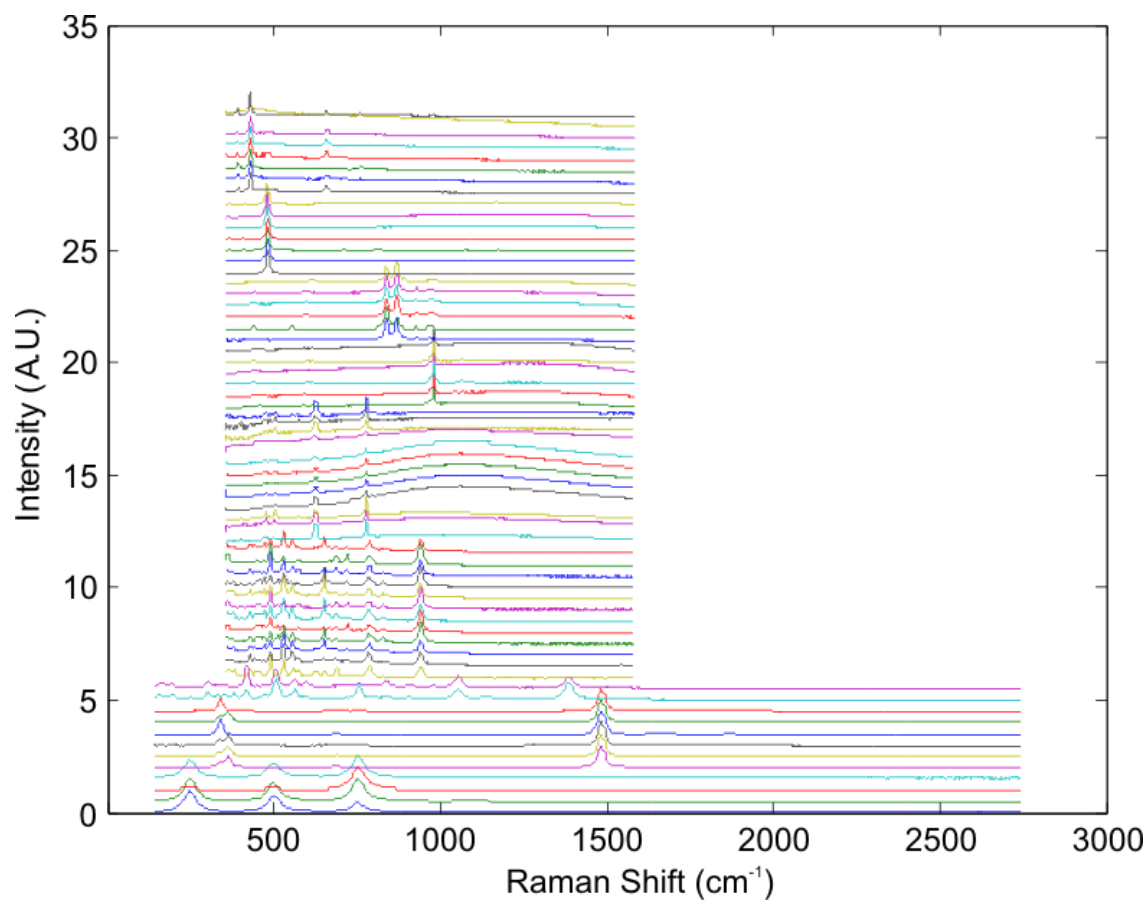
Vertical lines radiate using the automated SIM-based algorithms.

The peaks scoring above the SIM threshold are kept for the spectral identification. The SIM threshold score used here was 0.87. The peaks that have met the threshold level are shown in Fig. 17. The plot in Fig.17 shows the Lorentzian band replacement spectrum. The Lorentzian band replacement peak intensities are the nominal intensities obtained from the difference between the original peak heights down to the baseline of the spectrum.

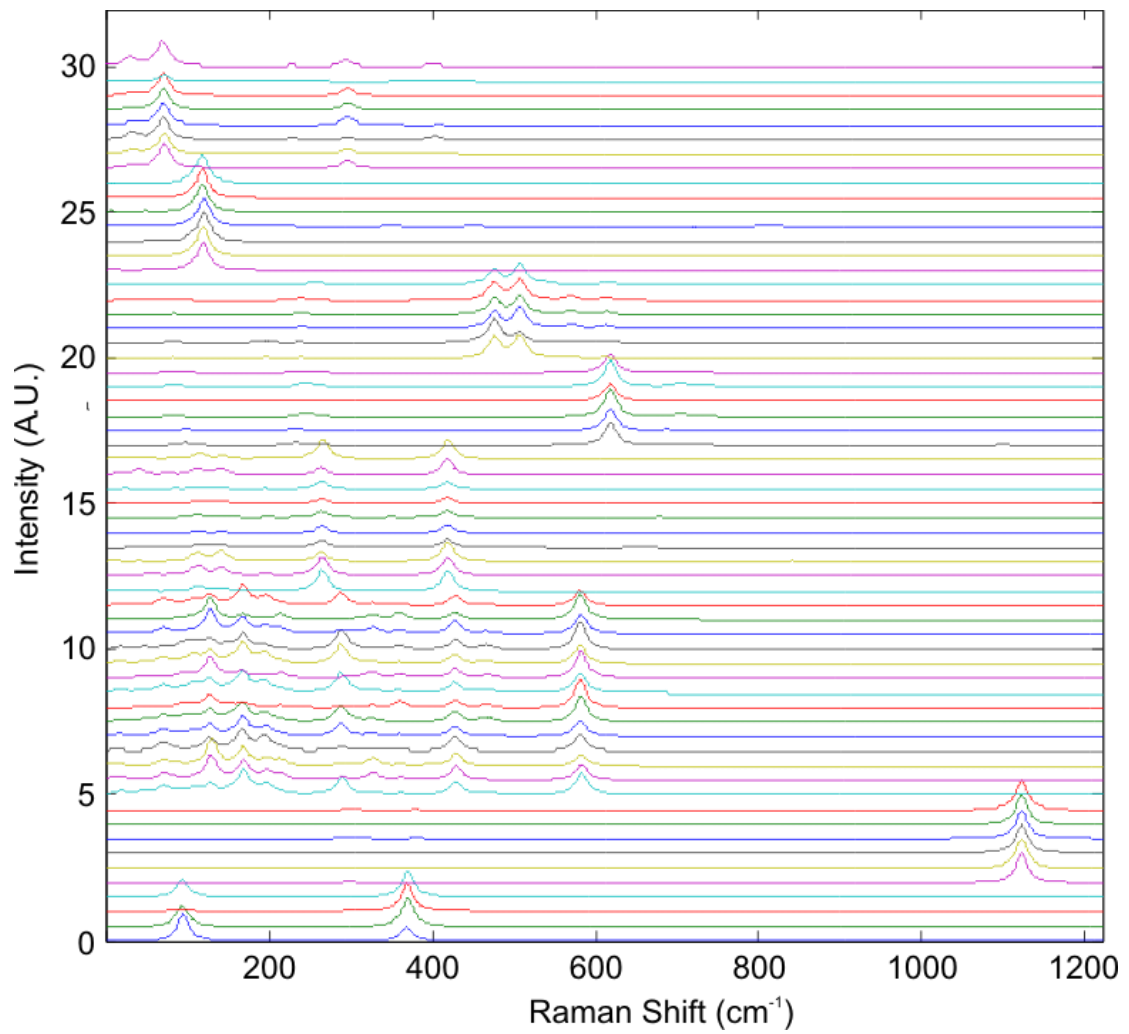


**Figure 17: Lorentzian Band Replacement of the Spectrum** a) Vertical lines indicates peaks found using the automated SIM-based computer algorithm.

All of the spectra analyzed by the procedure used here are given in Fig. 18. Some of the spectra extend farther than others. A common spectral range routine adjusts all the spectra so that all the pixel ranges are the same. Care should be taken if the ranges are non-linear or if the identifying spectral features are not in the analytical spectral range (i.e. the cut off largest peak intensities).

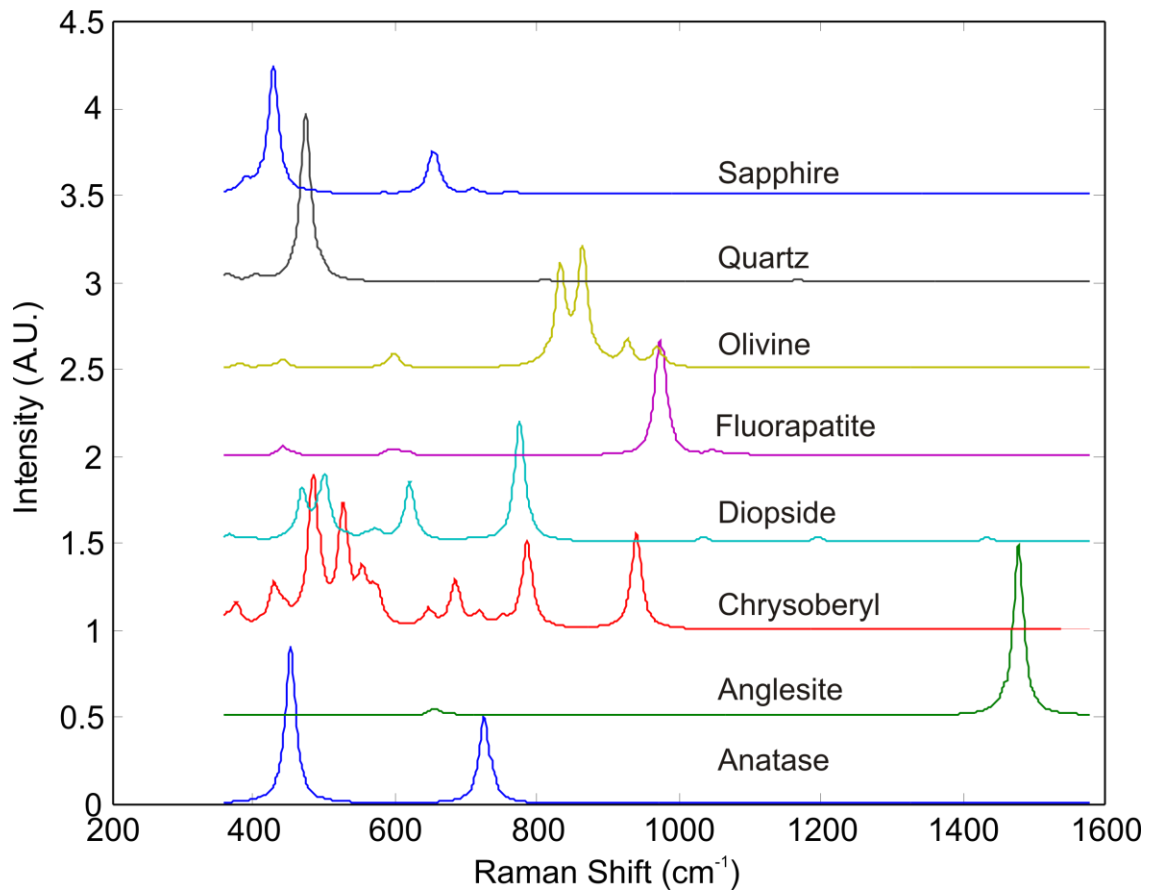


**Figure 18: Un-calibrated Raman Spectra of Mineral Dataset**



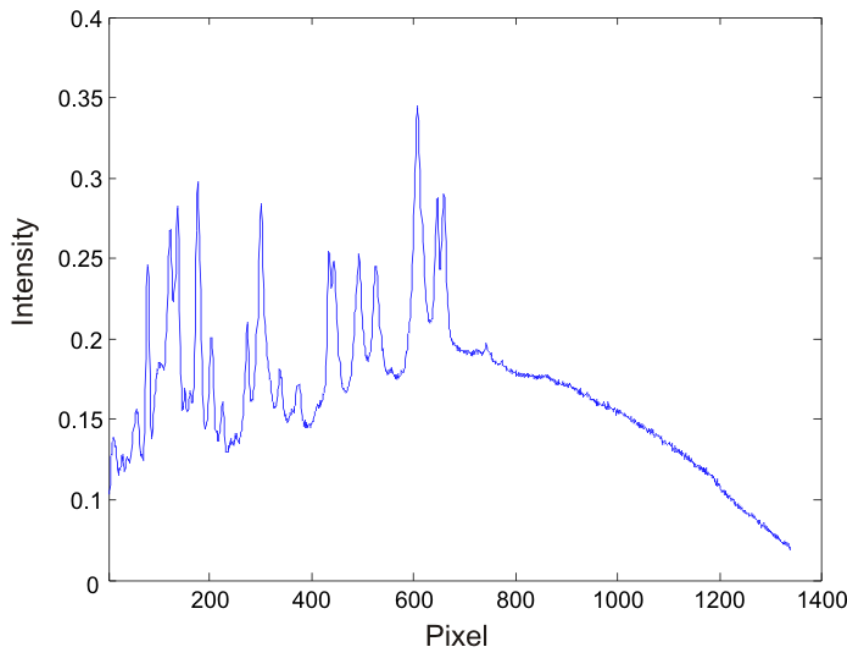
**Figure 19: All the Data in a Common Pixel Range**

All of the spectra are shown in a common range in Fig.19. The Lorentzian band replaced spectra for each mineral type are shown in Fig.20.

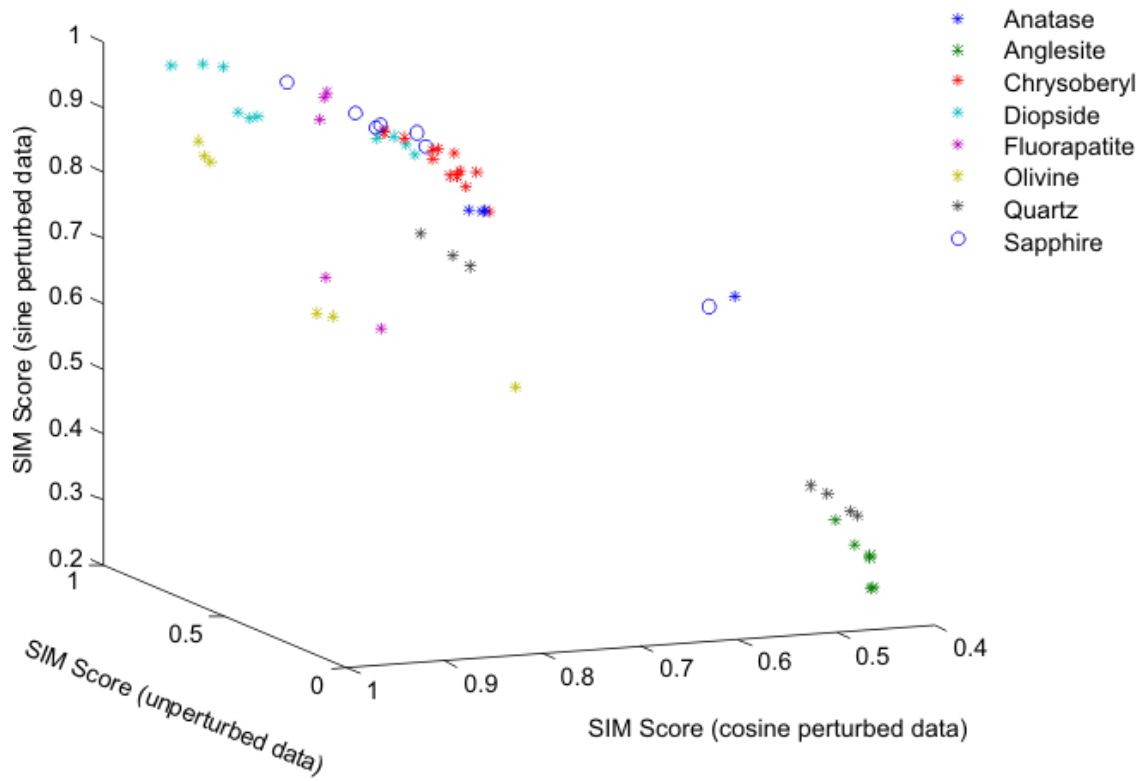


**Figure 20: Lorentzian Band Replaced Mineral Spectra**

Finally, three SIM scores are obtained for all the spectra. The reference vector is an average of all the spectra. The average reference spectrum is shown in Fig. 21. The three SIM scores are cast into three dimensions with each axis representing a SIM score value. All the scores are shown in appendix B. Figure 22 is a plot of the raw data scores and Fig. 23 is a plot of the Lorentzian band replaced scores. Figure 23 shows a tighter clustering of the data with fewer possible overlaps when compared to Fig.22.

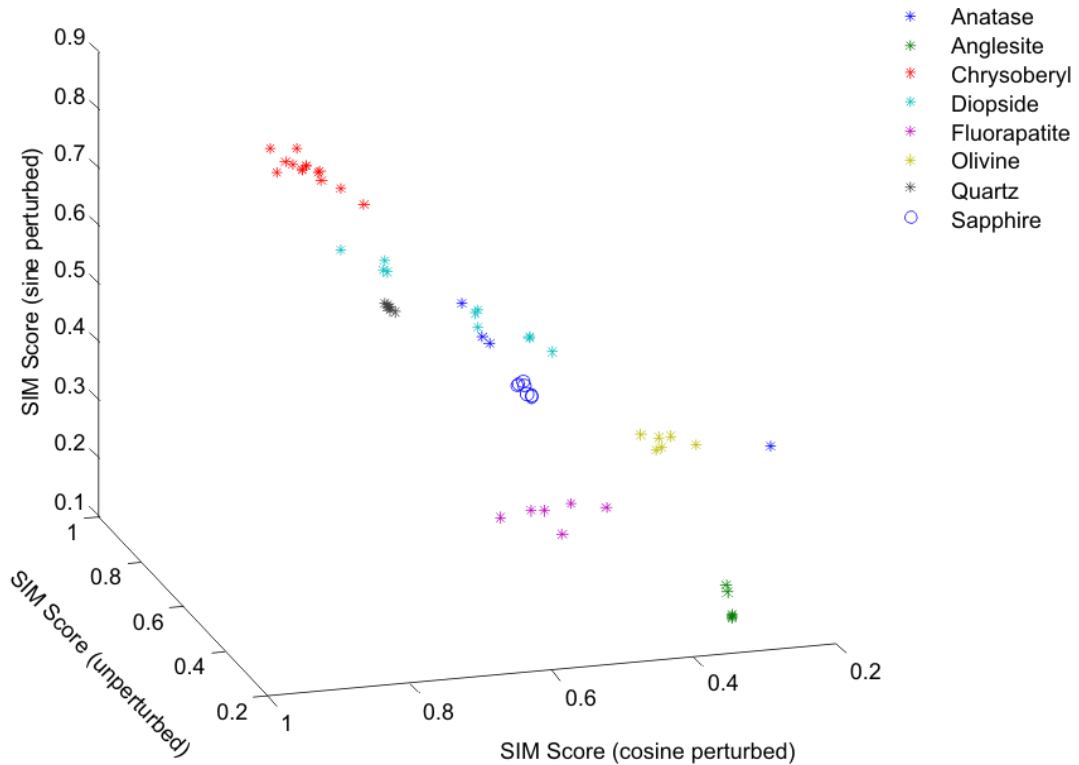


**Figure 21: Average Reference Spectrum**



**Figure 22: Cluster Plot of SIM Scores**





**Figure 23: Cluster Plots of Lorentzian Replacement Band SIM Scores**

#### 4.2 Statistical Comparison of the SIM Results

A statistical data analysis was performed in order to determine how well the SIM method was able to differentiate the sample spectra. Different dataset sizes were involved.

The descriptive sample statistics for the SIM scores are listed in appendix C. ANOVA testing using Minitab<sup>®</sup> was used to differentiate the SIM scores for the raw data and the Lorentzian band data. The ANOVA results are shown in appendix D for each sample pair. A summary table for appendix D results is shown in table II.

The ANOVA testing performed here gives the 95% confidence results that the samples are not the same. The ANOVA summary table is marked with “NO” if the samples were determined not to be the same. A “YES” is displayed if the individual

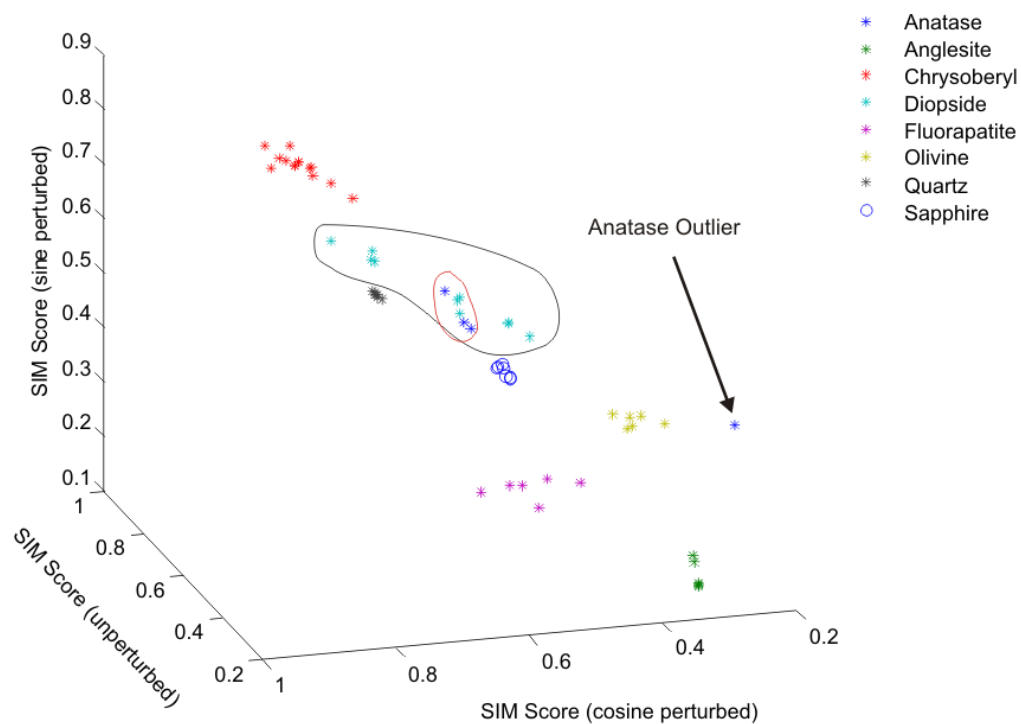
SIM values are statistically indistinguishable. If all three SIM values are indistinguishable the samples can be considered potentially the same.

The only samples potentially identified to be the same here, after the Lorentzian band replacements, are Anatase and Diopside. Further inspection of the plotted SIM values show that the values for Anatase and Diopside lay very close to one another. However, Anatase and Diopside are shown as visually distinct clusters in Fig. 24. Additional differentiating techniques should be used for these samples and any other potential cluster overlaps.

**Table II: Summary table of ANOVA for SIM Values**

ANOVA SIM Results							
SIM cos values							
SAMPLE	Anglesite	Chrysoberyl	Diopside	Fluorapatite	Olivine	Quartz	Sapphire
Anatase	NO	NO	NO	NO	NO	NO	NO
Angelsite		NO	NO	NO	NO	NO	NO
Chrysoberyl			NO	NO	YES	NO	NO
Diopside				NO	NO	NO	NO
Fluorapatite					YES	NO	YES
Olivine						YES	YES
Quartz							NO
ANOVA SIM Results							
SIM coscos values							
SAMPLE	Anglesite	Chrysoberyl	Diopside	Fluorapatite	Olivine	Quartz	Sapphire
Anatase	NO	NO	NO	NO	NO	YES	YES
Angelsite		NO	NO	NO	NO	YES	NO
Chrysoberyl			NO	NO	NO	NO	YES
Diopside				YES	YES	NO	YES
Fluorapatite					YES	NO	YES
Olivine						NO	NO
Quartz							NO
ANOVA SIM Results							
SIM sincos values							
SAMPLE	Anglesite	Chrysoberyl	Diopside	Fluorapatite	Olivine	Quartz	Sapphire
Anatase	NO	NO	NO	YES	YES	NO	YES
Angelsite		NO	NO	NO	NO	NO	NO
Chrysoberyl			NO	YES	NO	NO	YES
Diopside				YES	NO	NO	YES
Fluorapatite					YES	NO	YES
Olivine						NO	NO
Quartz							NO
ANOVA SIM Lorentzian Band Replacment Results							
SIM cos values							
SAMPLE	Anglesite	Chrysoberyl	Diopside	Fluorapatite	Olivine	Quartz	Sapphire
Anatase	NO	NO	YES*	NO	NO	NO	NO
Angelsite		NO	NO	NO	NO	NO	NO
Chrysoberyl			NO	NO	NO	NO	NO
Diopside				NO	NO	YES	NO
Fluorapatite					NO	NO	NO
Olivine						NO	NO
Quartz							NO
ANOVA SIM Lorentzian Band Replacment Results							
SIM coscos values							
SAMPLE	Anglesite	Chrysoberyl	Diopside	Fluorapatite	Olivine	Quartz	Sapphire
Anatase	NO	NO	YES*	YES	NO	NO	NO
Angelsite		NO	NO	NO	NO	NO	NO
Chrysoberyl			NO	NO	NO	YES	NO
Diopside				NO	NO	NO	NO
Fluorapatite					NO	YES	YES
Olivine						NO	NO
Quartz							NO
ANOVA SIM Lorentzian Band Replacment Results							
SIM sincos values							
SAMPLE	Anglesite	Chrysoberyl	Diopside	Fluorapatite	Olivine	Quartz	Sapphire
Anatase	NO	NO	YES*	NO	NO	NO	NO
Angelsite		NO	NO	NO	NO	NO	NO
Chrysoberyl			NO	NO	NO	NO	NO
Diopside				NO	NO	YES	NO
Fluorapatite					NO	NO	NO
Olivine						NO	NO
Quartz							NO

YES = statistically indistinguishable at 95% CI, check all the data to observe sample difference  
 NO = statistically not the same  
 \*Refer to the appendix for F statistics and P-values  
 Anatase Outlier #3 Removed



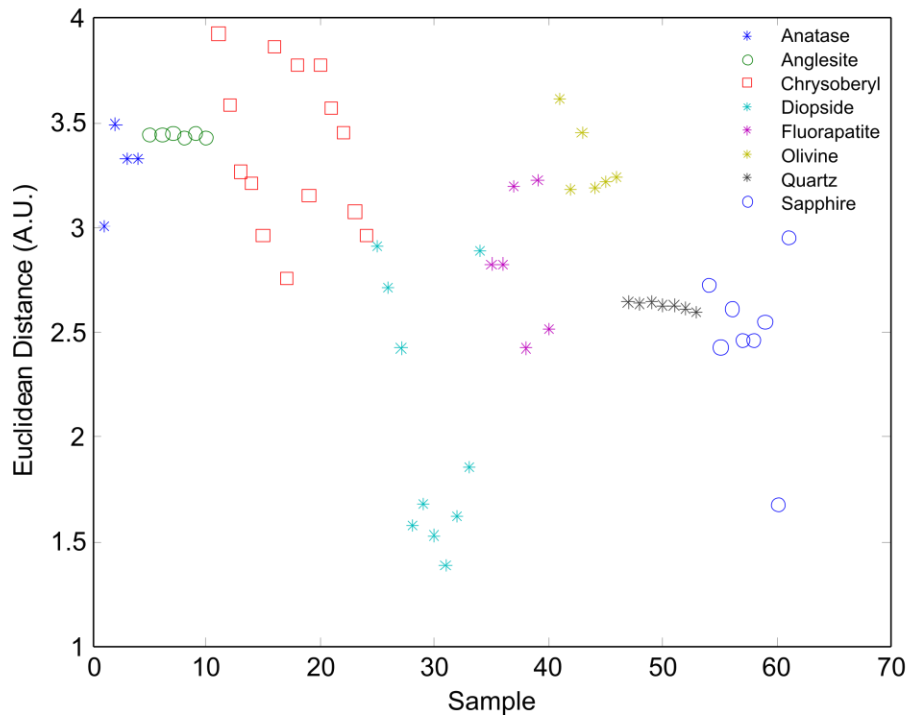
**Figure 24: Cluster Overlap with SIM Results** a) Potential overlap of Anatase with Diopside.

Additional differentiating techniques could include better choices of reference vectors and clustering analysis techniques. Alerts, scoring and data presentation to the analyst can also be used to distinguish potentially similar results. Referring back to the raw SIM values, the Anatase and Diopside clusters appear distinct also. The sample sets used here were only to demonstrate identification efficacy of SIM in the absence training data and using a very poor reference vector. Larger sample sets would probably provide better statistics for sample identification. Pooled standard deviations of the SIM results are listed in appendix D.

### 4.3 Euclidean Distance Measurements

In order to further demonstrate the effectiveness of SIM, a comparison with distancing methods is performed. Euclidean distance measures the distance of a sample vector from a reference vector. The closer a sample vector is to the reference vector, the smaller the Euclidean distance. Samples that are similar will produce similar Euclidean distances forming group clusters.

The general form of the Euclidean distance was previously given in Eq. 8. Fig. 25 is a plot of Euclidean distance results for the mineral data used in the SIM procedure.



**Figure 25: Euclidean Distance Results**

The Euclidean distance results were based on unit reference vector data. Results for each sample can be determined from plot by drawing a horizontal line

through the samples. The Euclidean distance results show overlaps with some of the values when using an average spectrum as the reference vector for all the data. Also, the values would normally *not* be color coded if they were unknowns. Without the color coding Fig. 25 would clearly depend on other analysis techniques to differentiate the samples.

The average reference vector represents the worst case scenario. An optimized reference vector would be preferable for measuring the Euclidean distance. A reference vector optimization, would take more time for calculation and judgment from an analyst.

#### 4.4 Mahalanobis Distance Measurements

Mahalanobis distance measurements are scale invariant. They can identify whether a sample belongs to a group based on group variance about a mean value, usually as a normal distribution. In addition, covariance with other measurement parameter can be investigated to help differentiate sample groups based.

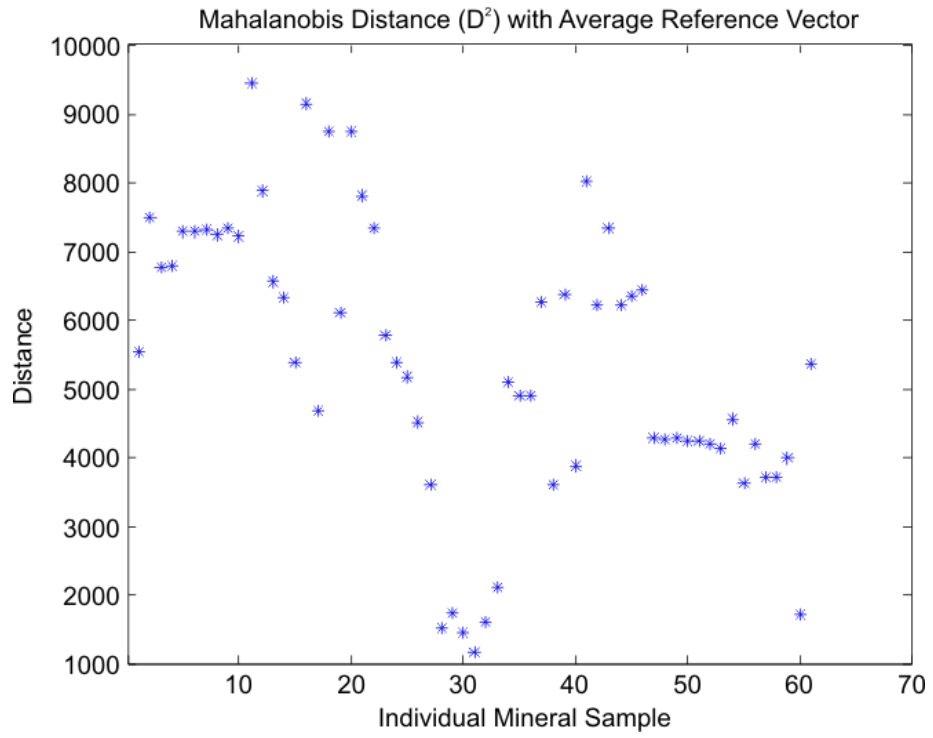
Mahalanobis measurements were calculated for the sample here following the general Mahalanobis formula given in Eq. 9.

$$D_M = \sqrt{(x - \mu)^T S^{-1} (x - \mu)} \quad (9)$$

In Eq. 9,  $x$  is the sample matrix vector,  $\mu$  is a matrix of means for reference group dimensions and  $S^{-1}$  is the covariance matrix for the reference group dimensions, excluding the sample to be measured.

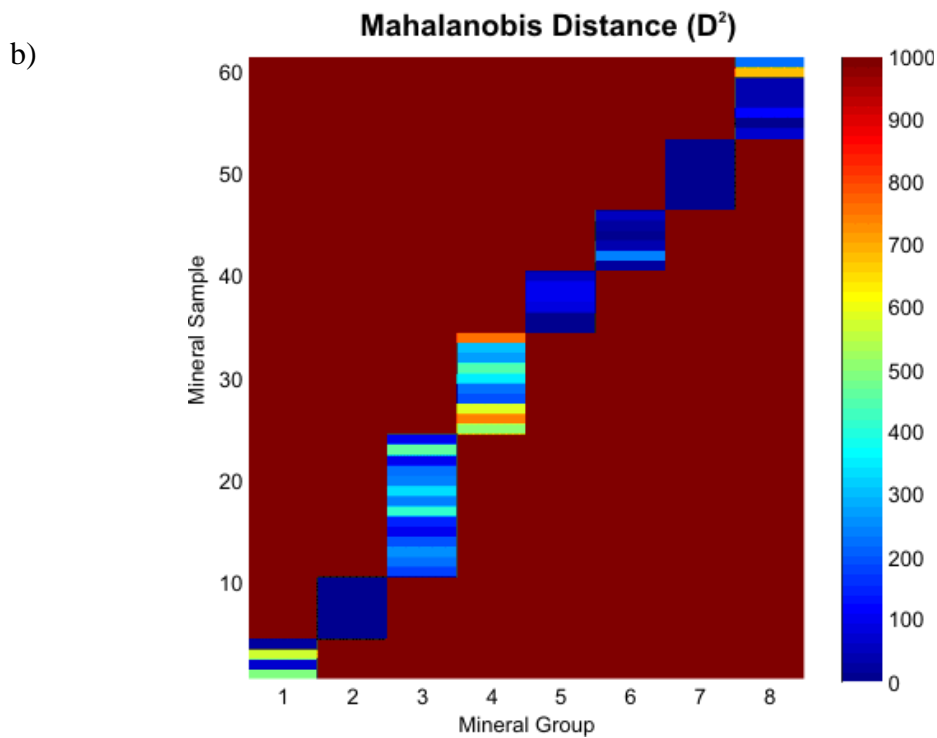
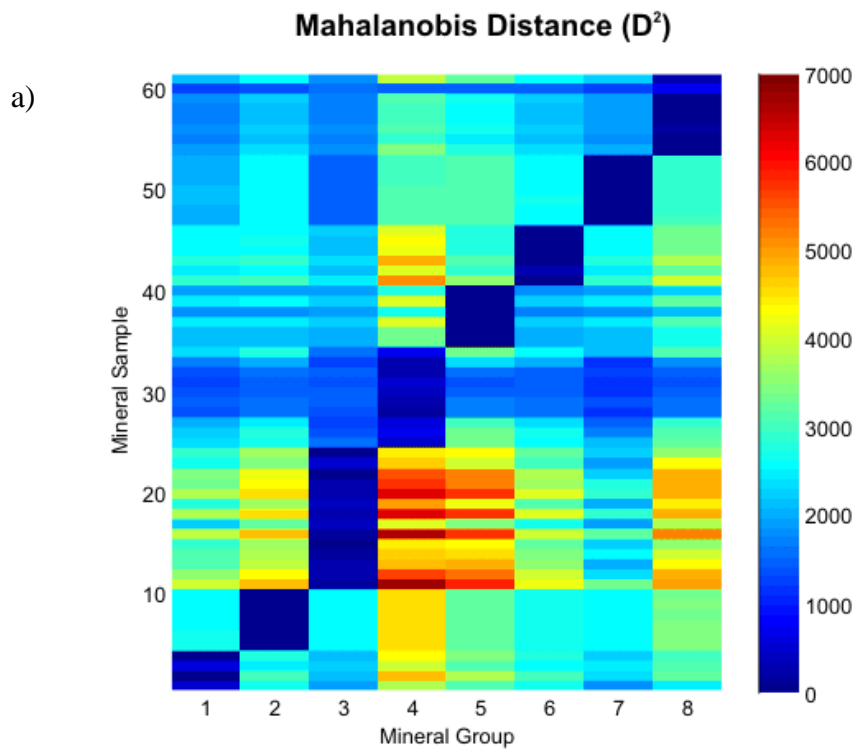
The Mahalanobis distance results calculated with an average reference vectors are given in Fig. 26. The individual sample groups are nearly indistinguishable with the average reference vector used for all the samples when the points are plotted as unknowns. These results show a similar distribution as the Euclidean distance results in Fig. 25.

The Mahalanobis distance results for the mineral dataset with one set of optimized reference vectors are given in Fig. 27. A table of the results is given in appendix F. The Mahalanobis distance was calculated for each sample to each mineral group in order to identify which group the sample belonged to, while generating contrast to the other groups. Fig. 27a is an image matrix of the results. The image matrix shows the mostly likely group each sample belongs to with a color scale. The Mahalanobis distances are closer to 0 if the sample is likely to belong to a particular mineral group. This is indicated by a deep blue color. Fig. 27b shows the Mahalanobis distances with an adjusted color map scale. Fig. 27b shows more contrast for the samples. The increased contrast in this image shows potential outliers for each mineral sample group.



**Figure 26: Mahalanobis Distance with an Average Reference Vector for All the Samples**





**Figure 27: Mahalanobis Distance Results with Optimized Reference Vectors** a) Distance results with normal color map scale and b) one-seventh scale results for contrast. (See Table VI in Appendix F)

## CHAPTER V

### SUMMARY, CONCLUSION AND RECOMENDATIONS

#### 5.1 Summary

A protocol used to calibrate, identify and database Raman spectra was developed here. It has been shown that spectral identity mapping (SIM) is capable of advanced spectral analyses due to the ability to identify spectral features through spectral matching. The work outlines the implementation of SIM for Raman spectra calibration, a method for data classification and analysis, and how to make the data and analysis protocols available to the public (see appendix A).

Variations in the instruments can make analyses difficult. Previous work utilizing SAM, CCA and other methods can suffer from many factors making analyses difficult. Data analysis can require a significant amount of time by the analyst for identification of unknowns. Even when identified, significant variations within the data may exist. Methods like Euclidean distance can provide unclear results if reference vector optimization is not performed. The method does not account for variance in the data. The Mahalanobis method is scale invariant, but relies on training data sets. SIM provides solutions to these problems in the form of matrix base algorithms that are scale invariant, have the ability to differentiate spectra even when using a poor reference vector and is easily automated for large data sets.

## **5.2 Conclusion**

Using developed algorithms and protocols, methods to calibrate Raman spectra, identify the spectra and to make the spectra available to a wide audience were created. This work focused on the use of multispectral algorithms utilizing SIM. Protocols for disseminating the algorithms and calibrated data were illustrated (appendix A). Multiple mineral data classes were tested in order to demonstrate the effectiveness of the SIM algorithms.

The SIM algorithm was able to satisfactorily calibrate the acquired data by taking into account daily variations of data acquisition with a calibration spectrum. The SIM algorithm was applied to several minerals and showed three dimensional data clustering. This was verified through ANOVA testing statistics. Finally, a referencing structure was developed utilizing databasing and web development software (appendix A).

## **5.3 Recommendations**

Despite all of the things developed to analyze and present the Raman data, there are still many ideas that should be explored for the processing and presentation of the data. A list of some additional work is presented below.

- Extend the spectral libraries with more materials
- Apply more visual descriptive statistical methods such as directional statistics to highlight sample contrast
- Expand Matlab algorithms in order to calibrate data not taken with similar equipment.

- Add web services for online calibration and search/matching.
- Develop device specific applications for processing offline mobile applications.
- Develop a database of user accounts to help manage the accessibility of features for the developers

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## **APPENDICES**

## **APPENDIX A:**

### **WEBSITE DEVELOPMENT**

#### **A.1 Introduction**

All of the code libraries described below are open source and can be configured or manipulated as the user desires. There are many ways to construct code for website development. The goal here was to achieve the desired website functionality as efficiently as possible. Please refer to the web pages in the appendix or any of the described code resources in order see the implementation of the functional features described in the following sections.

The problem of presenting well displayed, interactive Raman data to users/clients is scientifically challenging. Initially, all of the computer languages and processes involved can be underestimated by the non-computer scientist. There is a learning curve involved to understand and implement code.

Hopefully, the following will provide a strong grasp for the reader regarding the scientific computer programming foundation required for presenting sample data and how to communicate any data utilizing the widely accessible platforms provided through the internet.

Security is very important to control the integrity and the flow of data for the website. Server access should be coded, as well as database access. The most basic security features described during server installation were instituted. References to the

security protocols are given with the server software. It is encouraged that additional security features be pursued for user/client and data protection.

Web pages are used to communicate information to the world. In order to develop web pages for this project no software installation is needed. Surprisingly, any webpage file can be created initially as a text file with the proper formatting and file extensions.

The communication standards are included in the head section of the webpage text documents. Basic elements or “tags” serve as HTML delimiters providing the browser with interpreting instructions for the text.

The tags are generally in pairs. An example for a page division is an opening delimiter `<div>` and a closing delimiter `</div>`. This format provides a container for content. Within the HTML file, deprecated (outdated) tags should be avoided if possible to prevent pages from becoming incompatible with new browser releases.

Division of code sections in the text/html files is necessary to maintain organization and functionality of document elements. There are many tag elements given in the references that help achieve well written documents.

If any future work is performed to reconfigure website files, it should be determined what element usage is important to sending the information and what the user is trying to achieve. Cross browser functionality is very important. Finally, all HTML pages should be saved with the extension “.htm” or “.html”. These extensions let the browser recognize the files as web content. This can change depending on alternative server usage.

The brief HTML overview given is to help show that the HTML language is basically a structural language for how web pages are communicated and developed.

There are many other features that can be added in order to communicate various types of information and portray the information in a way that make it appealing, as well as educational to the reader.

Once code has been written for web pages, it is suggested that all code be tested for all possible mediums that may handle the code for the maximum user accessibility. In addition, even though files maybe generated in any text writer, the need to debug scripts (code/html files) begs for the use of more advance program writing environments.

There are many development environment programs available. They can be found for free performing an internet search for the specific programs. However, many of these are not yet compatible for all code/language combinations. There can also be significant challenges when trying to setup development environments for a specific developer, let alone trying to observe the interaction of the web pages with one another.

The environment utilized for developing this site was the most up to date Mozilla Firefox<sup>®</sup> browser and the Firebug<sup>®</sup> extension. Firebug<sup>®</sup> allowed fast detailed viewing of the data exchanged between the website server and browser. Another good development environment is Eclipse<sup>®</sup>, but it can be overwhelming for a novice script writer. There are many Eclipse<sup>®</sup> plug-ins available to help create a custom development environment.

Finally, although scripts can also be developed in a text writer without any additional software, graphing tools and widgets require reference to proprietary functional libraries. The choices of these are dependent of the development goals. The ones used here are described in detail below and with full scripts in the appendices.

## A.2 HTML/Internet Standards

The primary languages used to develop the web pages for this project were HTML/CSS. There are many other data exchange methods available including MIME, CGI, XML and Perl scripting. The information for all of the content for the web page is described by the “markup” of the information written in a text/html document, making it universally accessible.<sup>36</sup>

HTML has three principal types of markups: elements, attributes, and values.<sup>36</sup> Elements describe the structure of the different parts of the web pages. Attributes contain information about the data for the web pages and are described by values given by the programmer/user. Resources with listings of elements, attributes and possible values, along with how they are utilized can be found all over the internet by performing internet searches, reading forums or viewing the source code of a web page document. A comprehensive resource is [www.w3schools.com](http://www.w3schools.com).<sup>37</sup>

Browser interpretation of the text/html document information is critical to performance. In order to help achieve universal interpretation, character formats are employed. The character format suggested to be used is the Unicode character format, UTF-8.<sup>36</sup> Additional standards exist for the composition of web pages and should be declared for browser interpretation.

The standards are based on W3C consortium consensus and all statements for declaration of standards for this project are gathered from the training title HTML, XHTML, & CSS, Sixth Edition: Visual QuickStart Guide by Elizabeth Castro.<sup>36</sup>

At the time of writing this document, the standards used for the website are the most up to date. It is suggested that any possible standards updates be investigated and

referenced at <http://www.w3.org/standards/> or any other reliable source in order to achieve the optimal compatibility/operation of developed web pages.<sup>36</sup>

### **A.3 Website Communication**

Server/client software is required to exchange data. If additional server programs are added for other services, please be aware that communication problems can arise if the same computer port is used by two different server programs.

Individual operating system configurations must be made for server software to function properly. Please refer to operating system documentation for security settings in order to allow communication. Finally, the network security settings must be properly configured in order to allow data exchange requests.

Most websites use outside services for hosting due to the need for a static IP (internet protocol) address, high server speed and help with server configuration issues. If a local network is used, the administrator should have configured settings that allow communication to the server computer. If a domain name is used it must be registered in order to grant rights the namespace. There are several online service websites that can do this for a variety of fees. Free domain names are usually not in the familiar address bar formats.

Web pages are dynamic due their ability to reference data and files from one web page/script to another. This is done by the use of file calls, links and variables through the usage of powerful script languages. This basic concept is implemented through the use of a tool called the “uniform resource locator” (URL). The URL for a website helps a browser locate files and is used by high level software applications.<sup>36</sup>

The URL used to develop a website depends on the physical computer and location of the server software used to deliver website information to the user. While developing a website locally using server software, the URL will change to reflect the local computer used. The URL is simply a way to communicate where a file is located in the server directory.

The server setup is described within the server configuration instructions, initialization and configuration files. The URL prefix used is given below.

```
http://127.0.0.1/XXX or http://localhost/XXX (where XXX can be any file name)
```

#### **A.4 CSS**

One of the web page development tools used to make information appealing to the reader is called “cascade style sheeting” (CSS). Web pages are greatly enhanced with the use of .css files. CSS information can be developed within the HTML file or in a separate .css file and linked into existing HTML files using the linking procedure.<sup>36</sup> A typical .css markup (configuration) for an html the file shown below.

```
h1 {color: red};
```

There are three main components of CSS markup the selector, property and value.<sup>36</sup> The selector (above “h1”) defines which HTML elements are affected by the property and value within the brackets. The website visual appearance code can be separated from the structural code in the corresponding .html file allowing improved functionality when developing pages.

Appearances across pages can be quickly changed by making adjustments to .css files. The CSS pages are linked to the HTML pages with a formatted links in the header section. An example is given below:

```
<link rel="stylesheet" href="C:/xampp/htdocs/html/example.css" type="text/css" />
```

When using the selector format within the HTML page the `<style></style>` tags must be used to delimit all the selectors. CSS is mostly a static and structural language. Some dynamic effects can be produced with it and techniques can be found throughout the internet.

A better way to make pages more dynamic utilizes scripting language like PHP, JavaScript, JQuery and Flashmedia. Object oriented program languages like Visual Basic and Visual C may be used also, but they were not used here.

### **A.5 Ifranview**

In order to prepare the favicon for the pages an image can be developed in any preferred image development software. The image must be saved with an “.ico” extension. The Ifranview software is free and allows easy conversion of an image. Other graphical development software can be used, but some may charge for additional formats and professional versions that save graphics files properly. The Ifranview website is <http://www.irfanview.com/>.<sup>38</sup>

### **A.6 XAMPP/PHP**

HTML forms are used to communicate information to the world. There is only so much information that can be processed and stored efficiently in HTML pages. An additional program language used to handle data for the website here is pre-hypertext transfer protocol (PHP).

The version of PHP used here was derived from the free Apache<sup>®</sup> software and was packaged along with website management software in the XAMPP package. The



package for a particular operating system can be found at

<http://www.apachefriends.org/en/xampp.html>.<sup>39</sup>

This package contains all the server software needed to efficiently operate a data driven website. Even though file development can be straightforward, uploading and installation of functional server packages can be cumbersome. It is suggested that developers *carefully* install whatever server packages are needed. There are many PHP packages available and some require payment for usage.

A detailed text covering the capabilities of PHP is PHP 5 Unleashed by John Coggeshall.<sup>40</sup> There are many other PHP resources including the PHP developer's network forum located at [www.php.net](http://www.php.net).<sup>41</sup> It is suggested that the PHP version used is the most up to date in order to ensure that browser compatibility carries forward with site development.

PHP, like HTML and CSS, is a scripting language mainly meaning that it is interpreted as written and not compiled for operation like other programs. PHP is interpreted at the server hosting the webpage. PHP scripts can be started within HTML files using the PHP the delimiter “<?PHP” at the start of instruction and “?” at the end of instructions.

Scripts created using PHP within HTML may contain all the typical code elements/input fields used to gather information from a visitor. Form elements have been used here for the search and spectra data file retrieval sections of the webpage.

An important feature of PHP is the ability to create developer defined functions. For the most part, defined functions were intentionally avoided here because their functionality can be unclear in the context of website operation for new programmers.

There are many built-in functions that help to make scripting operations as efficient as possible. They can be found in the resources previously given.

### **A.7 PHP/SQL/phpMyadmin Database Management/RegEx**

In order to be able to take advantage of the PHP information processing abilities a database server is packaged with the PHP libraries and is preconfigured in XAMPP. There are many other proprietary languages used to manage data with a database in a website. The one used here is Structure Query Language (SQL). MySQL<sup>®</sup> is the program library utilized and SQL can be directed from PHP, the command prompt or other management applications. The database management application used here was phpMyadmin and is package within XAMPP.

There are both text and online resources for learning to program with SQL and the functions of phpMyadmin<sup>®</sup>. Resources used to learn this management program were [http://www.php-editors.com/articles/sql\\_phpmyadmin.php](http://www.php-editors.com/articles/sql_phpmyadmin.php) and “PHP for the World Wide Web” by Larry Ullman.<sup>42,43</sup> This combination of resources covers everything necessary to produce a functional data driven web page with the accessibility to website data.

Using SQL allows the website to provide more efficient information exchange to site users. PhpMyAdmin provides a web interface for administering SQL databases. Operation details are given by Marc Delisle.<sup>44</sup> PhpMyAdmin<sup>®</sup> offers features that cover basic MySQL database and table operations. It can manage metadata to support many advanced features.<sup>44</sup>

Some of many features available for handling data in phpMyAdmin<sup>®</sup> given by Delisle are listed below.

- Database creation and manipulation
- Information Editing
- Simple Navigation and Search Functions

The phpMyAdmin<sup>®</sup> server administration features also consists of many user privilege features.

Within PHP scripts there are many tools and formats a user can use to connect to a database server. In order to utilize database server functionality within a PHP script you have to create the database and establish a connection to the database server.

There were two ways used here to create the databases utilized here. The first was with phpMyAdmin<sup>®</sup> and the second with PHP scripting. The following command within a PHP script can be used:

```
CREATE DATABASE database_name
```

A database connection will then be needed as the access point for any future data retrieval commands. The MySQL syntax for connecting to a database is:

```
$Link = mysql_connect ("host", "user", "password");
```

A link is established by using three arguments: host, which is almost always localhost described by the server IP address, username and password for that user name. The last two parameters will dictate what database permissions you have. Different users will have different access controls to the database server depending on its configuration.

Finally, you can query through the connection utilizing

```
mysql_query ("databasename", $Link);
```

The \$Link value is established when connecting to a database and is used to continue working with the database.<sup>44</sup> The following command closes a link:

```
mysql_close($Link);
```

Attached as an appendix are the PHP script files using these commands in order to submit site request to the MySQL<sup>®</sup> databases. These requests are hyperlinked to the Raman database and information is retrieved during a user search/request.

Query searches range from simple to complex. There is an entire science behind efficient query searching. One language structure used to make searching more efficient within a query is “regular expressions”.

Both PHP and Java take advantage of regular expressions for performing searches of data. Please refer to the references above on how to incorporate regular expression into advanced data searches if they are warranted. A good online resource on the operation of regular expression is <http://www.regular-expressions.info/>.<sup>45</sup>

## **A.8 Java/JQuery**

Although the XAMPP package is sufficient for exchanging content with users, efficient element manipulation and page dynamics are not capable with PHP scripts alone. The scripting libraries used to help implement more fluid presentation of the data were Java and JQuery.

Java is a scripting language that utilizes the user computer processing instead of the server in order to manipulate data. Java libraries are typically built into most browsers and must be updated regularly. All Java updates are usually set to automatically update in modern browsers and the latest versions can be also checked at [www.java.com](http://www.java.com).<sup>46</sup>

JQuery<sup>®</sup> is web scripting language developed in order to make working with Java easier. JQuery<sup>®</sup> libraries and configuration are free and can be downloaded at [www.jquery.com](http://www.jquery.com).<sup>47</sup> The JQuery<sup>®</sup> forums for the site give very good instruction on

using the libraries. A detailed resource about JQuery<sup>®</sup> is JQuery in Action 2<sup>nd</sup> Edition by Bear Bibeault and Yehuda Katz.<sup>48</sup> This text contains a plethora of useful page applications.

JQuery<sup>®</sup> and Java typically are used to make widgets, dynamic programming mechanisms, and are referenced in the HTML pages by utilizing tags script tags similar to the ones below.

```
<script type="text/javascript"></script>
```

Scripts can be initiated at any point with the HTML file. The most important feature about running a script is the ready handler. Literature should be reviewed regarding ready handler implementation. The ready handler is the way the script recognizes when to operate within an HTML file. User defined functions can be defined within the script tag elements.

There are many free user defined JQuery<sup>®</sup> widgets available. They can be found by simple internet searches. Most have been avoided developing this website because they can pose challenges to operating properly with all the elements in a script.

## **A.9 Website Graphics / Highcharts**

The current group of free graphing packages available to present data to the user are lacking in advanced features. Graphing package can function from both the server side (PHP) and user side (Java) scripting languages. HTML graphics can be developed with a software package or simple HTML Canvas tags and the use of scalable vector graphics (SVG) elements. There are many HTML Canvas training titles available.

A highly functional graphing package is Highcharts<sup>®</sup>. The libraries for this package can be found at [www.highcharts.com](http://www.highcharts.com).<sup>49</sup> There are many interesting graphing

capabilities in Highcharts<sup>®</sup>. Highcharts<sup>®</sup> graphs can be difficult to implement from scratch. Fortunately, there are many samples that can be followed. Highcharts takes advantage of a development environment called jsFiddle<sup>®</sup> to demonstrate its capabilities. Please refer to the script pages to see how Highcharts<sup>®</sup> were implemented here or the website for many advance features.

The following is a list of how Highcharts<sup>®</sup> is used here in order to display the mineral spectra.

- Display single or multiple spectra together
- Display separate spectra in separate graphs for comparisons
- Display spectral data points
- Zooming in and out of spectral features
- Removal of unwanted spectral data

## **A.10 MediaWiki**

In order to make to the website more interactive and contributable, MediaWiki<sup>®</sup> was added as a blogging tool. There are many great blogging tools available. These tools make informational databases more of an “experience” for dynamic information exchange. MediaWiki is free package and can be found at [www.mediawiki.org/wiki/MediaWiki](http://www.mediawiki.org/wiki/MediaWiki).<sup>50</sup>

More time would have like to been taken to investigate the use of Drupal, Wordpress or to construct a simple PHP blog. MediaWiki is functionally similar to Wikipedia so usage should be familiar to a wide audience. MediaWiki consist of its own database software for managing community content and is included in the download. Please refer to the MediaWiki installation instructions for configuration.

The hope is that spectral data of all types can be submitted to this site and be both assigned and referenced to users for free. This could grow the database faster. A mechanism to submit larger amounts of data will probably need to be constructed, as well as tool for integrating data to the general website from the blogs.

## **A.11 Recommendations**

### **A.11.1 XML Data exchanges with PHP or Proprietary packages (Live Data Analysis Web Service)**

There are two main ways Matlab scripts can be administered to users over the internet. One way is through the use of a developed Java script widget. The second is a live processing of spectral data with a “web service”.

Proprietary Java Script-Java-Matlab interface commands can be used to produce real-time user non-assisted analysis of the Raman data acquired for field and web acquired data. The data can be submitted to the MySQL database adding to the collection of website data. Matlab help documents cover the procedures and resources to implement this “web service”.

In order to make Matlab script files available to webpage visitors in a widget, Matlab builder JA can be used to deliver specialized image analysis scripts. The package is not available in the student versions of Matlab. The professional Matlab version must be obtained to practice utilizing the Matlab script conversion package.

The package allows the deployment of Java enveloped scripts in two ways. Deployment can root from the server hosting the webpage or can be deployed to the user with accepted download of a specialized runtime package.

Dynamic data exchange can also be established utilizing extensible markup language (XML). PHP5 unleashed by John Coggeshall covers XML and there are

many dedicated resources to XML. Other potential dynamic data exchange languages include CGI and Perl.

### **A.11.2 Handheld Devices**

One of the aims of this project is to develop a foundation for the capability to access spectroscopy data with handheld devices. Databases have been developed that make accessing information by a variety of devices possible. Wireless application protocol (WAP) and wireless access language (WAL) can help expand local/remote accessibility. Simulator software is available for most handheld devices and can be used to test Web site performance for future devices.

### **A.11.3 Apps**

An “app” (short for application) is a separate programming entity designed for a specific, usually mobile, device. A SIM method app specific to any popular device would become welcome addition towards achieving widespread SIM accessibility.

Unfortunately, this would require time to develop due to device specific development environments and monetary cost. This is particularly a problem with Apple devices due to the development package cost, but it is probably worth a long-term investment. There are free development packages for Android operating system devices. Visual Basic and Visual C are free from Microsoft and specialized devices utilizing microcontrollers geared toward these languages would also be beneficial i.e. Basic Stamp, PIC, TTL, PLC and Aduino (Atmel).



#### **A.11.4 Additional Graphics**

Flashmedia website provides some of the most beautifully presented data and media available. The spectroscopy database would probably gain significantly with properly implemented touches of these media tool. Windows Presentation Foundation (WPF) is developing a large following for presenting rich environments for presenting information.

Unfortunately, significant time would be spent learning to utilize .NET server framework and Active Script Pages (ASP). Qt is another interest presentation format and can be tied to MATLAB utilizing C programming structures. It could be utilized with LCD and OLED modules for independently developed devices. Delphi should be investigated toward standalone GUI's also.

#### **A.11.5 Additional Server Packages**

It is recommended that other complete web site development packages be investigated in order to increase efficiencies and accessibility of the spectroscopic data. Ruby on Rails is another package that could be used for managing website development. Intensive searches would probably reveal many others. Use of Active Script Pages (ASP) and JavaScript Pages (JSP) should also be investigated.

## APPENDIX B:

Table III. SIM Values

Sample	SIM cos values	SIM coscos values	SIM sincos values	SIM lor cos values	SIM lor coscos values	SIM lor sincos values
Anatase 1	0.6261	0.7037	0.7698	0.5605	0.6189	0.5932
Anatase 2	0.6169	0.7070	0.7686	0.5218	0.6021	0.5501
Anatase 3	0.4894	0.4815	0.6352	0.3305	0.2540	0.3964
Anatase 4	0.6267	0.7193	0.7696	0.5112	0.5957	0.5400
Anglesite 5	0.2942	0.4274	0.3178	0.2633	0.3274	0.1325
Anglesite 6	0.2750	0.4132	0.2812	0.2654	0.3279	0.1403
Anglesite 7	0.2536	0.4006	0.2168	0.2651	0.3272	0.1363
Anglesite 8	0.2604	0.4014	0.2608	0.2727	0.3301	0.1748
Anglesite 9	0.2539	0.4001	0.2180	0.2642	0.3266	0.1344
Anglesite 10	0.2612	0.4014	0.2675	0.2758	0.3316	0.1859
Chrysoberyl 1	0.6639	0.6894	0.7591	0.7370	0.7646	0.7545
Chrysoberyl 2	0.7107	0.7068	0.8173	0.7432	0.7670	0.7661
Chrysoberyl 3	0.6767	0.7096	0.7993	0.7433	0.7648	0.7683
Chrysoberyl 4	0.7186	0.7326	0.8498	0.7031	0.7142	0.7208
Chrysoberyl 5	0.7707	0.7686	0.8731	0.7538	0.7819	0.7743
Chrysoberyl 6	0.6864	0.7245	0.8156	0.7568	0.8088	0.7853
Chrysoberyl 7	0.7153	0.7626	0.8715	0.7117	0.8348	0.7858
Chrysoberyl 8	0.6871	0.7162	0.8136	0.7531	0.7881	0.7703
Chrysoberyl 9	0.6724	0.6993	0.8181	0.7348	0.8059	0.7882
Chrysoberyl 10	0.6871	0.7162	0.8136	0.7531	0.7881	0.7703
Chrysoberyl 11	0.7086	0.7353	0.8374	0.7659	0.8285	0.8035
Chrysoberyl 12	0.7267	0.7257	0.8501	0.7684	0.7912	0.7996
Chrysoberyl 13	0.6960	0.7165	0.8462	0.6949	0.7509	0.7539
Chrysoberyl 14	0.7707	0.7686	0.8731	0.7538	0.7819	0.7743
Diopside 1	0.9249	0.8678	0.8814	0.4984	0.5420	0.5482
Diopside 2	0.9652	0.9382	0.9635	0.6099	0.7154	0.6432
Diopside 3	0.9249	0.8813	0.8924	0.5989	0.7122	0.6435
Diopside 4	0.8708	0.7344	0.8464	0.5369	0.6026	0.5891
Diopside 5	0.8646	0.7250	0.8364	0.4751	0.5174	0.5308
Diopside 6	0.8559	0.7166	0.8197	0.5380	0.6070	0.5853
Diopside 7	0.8718	0.7512	0.8470	0.6278	0.7076	0.6524
Diopside 8	0.9544	0.9081	0.9635	0.5119	0.5395	0.5463
Diopside 9	0.9499	0.8900	0.9591	0.6403	0.7665	0.6730
Diopside 10	0.9210	0.8612	0.8840	0.5249	0.6068	0.5662
Fluorapatite 1	0.8702	0.8110	0.8812	0.3543	0.5834	0.3127
Fluorapatite 2	0.8710	0.8105	0.8810	0.3510	0.5656	0.3125
Fluorapatite 3	0.7083	0.8457	0.6699	0.3467	0.4787	0.3074
Fluorapatite 4	0.8915	0.7985	0.9175	0.3312	0.5458	0.2767
Fluorapatite 5	0.6684	0.7983	0.5920	0.3531	0.5271	0.3174
Fluorapatite 6	0.8893	0.8013	0.9124	0.3503	0.6265	0.3079

Sample	SIM cos values	SIM coscos values	SIM sincos values	SIM lor cos values	SIM lor coscos values	SIM lor sincos values
Olivine 1	0.6357	0.8557	0.6228	0.3854	0.3895	0.3885
Olivine 2	0.4951	0.7037	0.5185	0.3838	0.3980	0.3845
Olivine 3	0.6716	0.8633	0.6215	0.4056	0.3877	0.3956
Olivine 4	0.8881	0.9301	0.8584	0.4045	0.3712	0.3961
Olivine 5	0.8672	0.9292	0.8395	0.4142	0.4109	0.4015
Olivine 6	0.8543	0.9256	0.8324	0.3838	0.3432	0.3885
Quartz 1	0.3105	0.4322	0.3576	0.5754	0.7088	0.5848
Quartz 2	0.2830	0.4157	0.3308	0.5837	0.7175	0.5932
Quartz 3	0.2773	0.4084	0.3257	0.5800	0.7138	0.5905
Quartz 4	0.3252	0.4443	0.3676	0.5809	0.7171	0.5901
Quartz 5	0.7725	0.6815	0.6570	0.5790	0.7156	0.5865
Quartz 6	0.8137	0.7211	0.7062	0.5816	0.7181	0.5895
Quartz 7	0.7872	0.6962	0.6733	0.5857	0.7201	0.5950
Corundum 1	0.7772	0.7267	0.8472	0.4653	0.5574	0.4698
Corundum 2	0.8277	0.7861	0.8975	0.4739	0.5685	0.4798
Corundum 3	0.7811	0.7340	0.8690	0.4614	0.5509	0.4640
Corundum 4	0.8011	0.7714	0.8764	0.4705	0.5579	0.4800
Corundum 5	0.8011	0.7714	0.8764	0.4705	0.5579	0.4800
Corundum 6	0.8089	0.7650	0.8793	0.4741	0.5649	0.4820
Corundum 7	0.8864	0.8405	0.9401	0.4658	0.5507	0.4647
Corundum 8	0.5103	0.5041	0.6201	0.4757	0.5602	0.4865

\*The average data spectrum was used as a reference vector.

## APPENDIX C:

**Table IV. Descriptive Statistics: SIM values anSd SIM Lorentzian Replacement Values**

Variable	Count	Mean	SE Mean	StDev	Variance
Anatase SIM cos	4	0.5898	0.0335	0.0671	0.0045
Anatase SIM coscos	4	0.6529	0.0572	0.1144	0.0131
Anatase SIM sincos	4	0.7358	0.0335	0.0671	0.0045
Anatase SIM lor cos	4	0.4810	0.0513	0.1025	0.0105
Anatase SIM lor coscos	4	0.5177	0.0880	0.1761	0.0310
Anatase SIM lor sincos	4	0.5199	0.0428	0.0855	0.0073
Anglesite SIM cos	6	0.26638	0.00640	0.01568	0.00025
Anglesite SIM coscos	6	0.40735	0.00449	0.01100	0.00012
Anglesite SIM sincos	6	0.2603	0.0158	0.0387	0.0015
Anglesite SIM lor cos	6	0.26775	0.00212	0.00518	0.00003
Anglesite SIM lor coscos	6	0.32847	0.000797	0.00195	0.000004
Anglesite SIM lor sincos	6	0.15070	0.00954	0.02338	0.00055
Chrysoberyl SIM cos	14	0.70649	0.00878	0.03285	0.00108
Chrysoberyl SIM coscos	14	0.72656	0.00666	0.02491	0.00062
Chrysoberyl SIM sincos	14	0.83127	0.00863	0.03228	0.00104
Chrysoberyl SIM lor cos	14	0.74092	0.00608	0.02275	0.00052
Chrysoberyl SIM lor cosc	14	0.78362	0.00837	0.03132	0.00098
Chrysoberyl SIM lor sinc	14	0.77251	0.00560	0.02094	0.00044
Diopside SIM cos	10	0.9103	0.0130	0.0410	0.0017
Diopside SIM coscos	10	0.8274	0.0270	0.0854	0.0073
Diopside SIM sincos	10	0.8893	0.0174	0.0550	0.0030
Diopside SIM lor cos	10	0.5562	0.0184	0.0582	0.0034
Diopside SIM lor coscos	10	0.6317	0.0277	0.0876	0.0077
Diopside SIM lor sincos	10	0.5978	0.0162	0.0512	0.0026
Fluorapatite SIM cos	6	0.8165	0.0410	0.1004	0.0101
Fluorapatite SIM coscos	6	0.81088	0.00734	0.01798	0.00032
Fluorapatite SIM sincos	6	0.8090	0.0575	0.1409	0.0199
Fluorapatite SIM lor cos	6	0.34777	0.00348	0.00853	0.00007
Fluorapatite SIM lor cos	6	0.5545	0.0206	0.0504	0.0025
Fluorapatite SIM lor sin	6	0.30577	0.00600	0.01470	0.00022
Olivine SIM cos	6	0.7353	0.0650	0.1591	0.0253
Olivine SIM coscos	6	0.8679	0.0356	0.0873	0.0076
Olivine SIM sincos	6	0.7155	0.0594	0.1454	0.0211
Olivine SIM lor cos	6	0.39622	0.00549	0.01346	0.00018
Olivine SIM lor coscos	6	0.38342	0.00964	0.02362	0.00056
Olivine SIM lor sincos	6	0.39245	0.00258	0.00632	0.00004
Quartz SIM cos	7	0.5099	0.0997	0.2638	0.0696
Quartz SIM coscos	7	0.5428	0.0558	0.1476	0.0218
Quartz SIM sincos	7	0.4883	0.0678	0.1794	0.0322
Quartz SIM lor cos	7	0.58090	0.00125	0.00332	0.00001
Quartz SIM lor coscos	7	0.71586	0.00139	0.00368	0.00001
Quartz SIM lor sincos	7	0.58994	0.00134	0.00354	0.00001
Sapphire SIM cos	8	0.7805	0.0402	0.1136	0.0129
Sapphire SIM coscos	8	0.7448	0.0360	0.1017	0.0103
Sapphire SIM sincos	8	0.8570	0.0348	0.0983	0.0097
Sapphire SIM lor cos	8	0.46965	0.00178	0.00504	0.00003
Sapphire SIM lor coscos	8	0.55855	0.00217	0.00615	0.00004
Sapphire SIM lor sincos	8	0.47585	0.00300	0.00847	0.00007

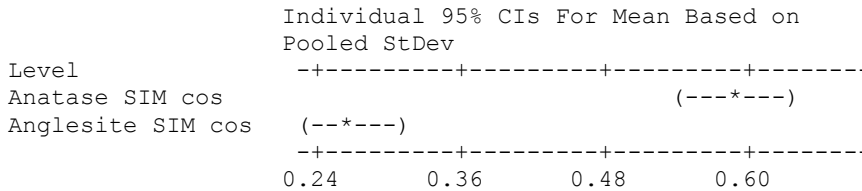
## APPENDIX D: One-way ANOVA Results

### One-way ANOVA: Anatase SIM cos, Anglesite SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.25100	0.25100	136.38	0.000
Error	8	0.01472	0.00184		
Total	9	0.26572			

S = 0.04290    R-Sq = 94.46%    R-Sq(adj) = 93.77%

Level	N	Mean	StDev
Anatase SIM cos	4	0.58977	0.06707
Anglesite SIM cos	6	0.26638	0.01568



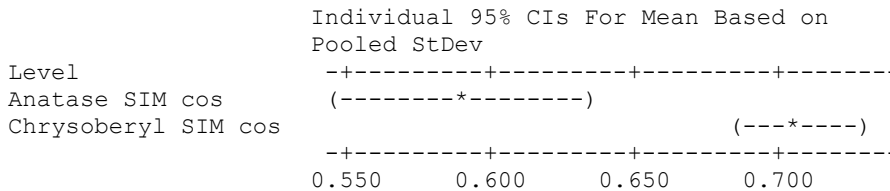
Pooled StDev = 0.04290

### One-way ANOVA: Anatase SIM cos, Chrysoberyl SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.04238	0.04238	24.64	0.000
Error	16	0.02752	0.00172		
Total	17	0.06991			

S = 0.04148    R-Sq = 60.63%    R-Sq(adj) = 58.17%

Level	N	Mean	StDev
Anatase SIM cos	4	0.58977	0.06707
Chrysoberyl SIM cos	14	0.70649	0.03285



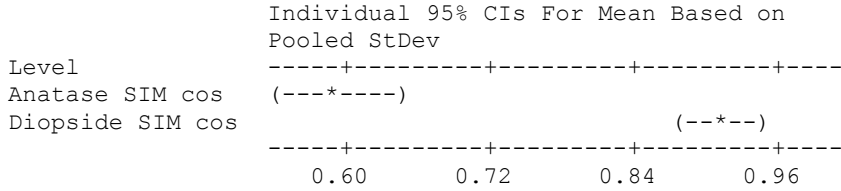
Pooled StDev = 0.04148

### One-way ANOVA: Anatase SIM cos, Diopside SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.29361	0.29361	122.97	0.000
Error	12	0.02865	0.00239		
Total	13	0.32226			

S = 0.04886    R-Sq = 91.11%    R-Sq(adj) = 90.37%

Level	N	Mean	StDev
Anatase SIM cos	4	0.58977	0.06707
Diopside SIM cos	10	0.91034	0.04104



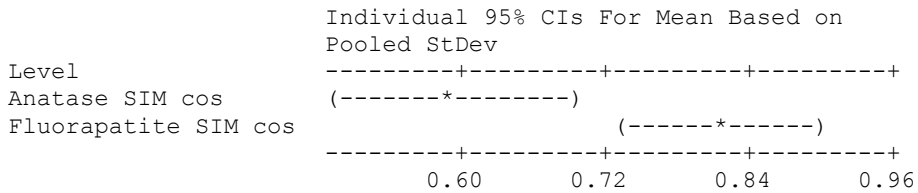
Pooled StDev = 0.04886

### One-way ANOVA: Anatase SIM cos, Fluorapatite SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.12332	0.12332	15.44	0.004
Error	8	0.06391	0.00799		
Total	9	0.18723			

S = 0.08938    R-Sq = 65.86%    R-Sq(adj) = 61.60%

Level	N	Mean	StDev
Anatase SIM cos	4	0.58977	0.06707
Fluorapatite SIM cos	6	0.81645	0.10042

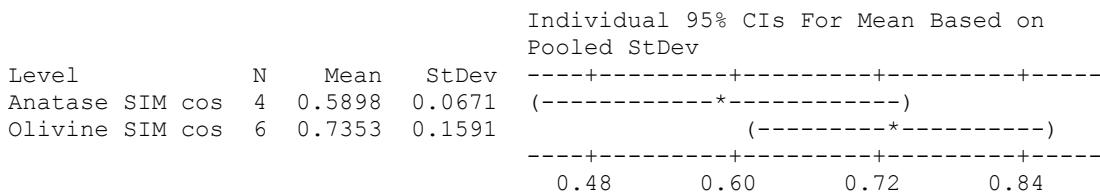


Pooled StDev = 0.08938

### One-way ANOVA: Anatase SIM cos, Olivine SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.0508	0.0508	2.90	0.127
Error	8	0.1401	0.0175		
Total	9	0.1909			

S = 0.1323    R-Sq = 26.63%    R-Sq(adj) = 17.46%

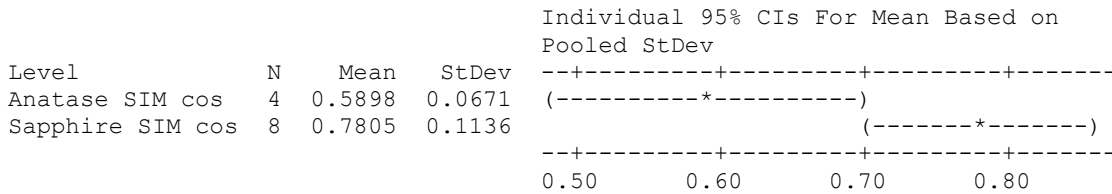


Pooled StDev = 0.1323

**One-way ANOVA: Anatase SIM cos, Sapphire SIM cos**

Source	DF	SS	MS	F	P
Factor	1	0.0970	0.0970	9.35	0.012
Error	10	0.1038	0.0104		
Total	11	0.2009			

S = 0.1019 R-Sq = 48.31% R-Sq(adj) = 43.14%

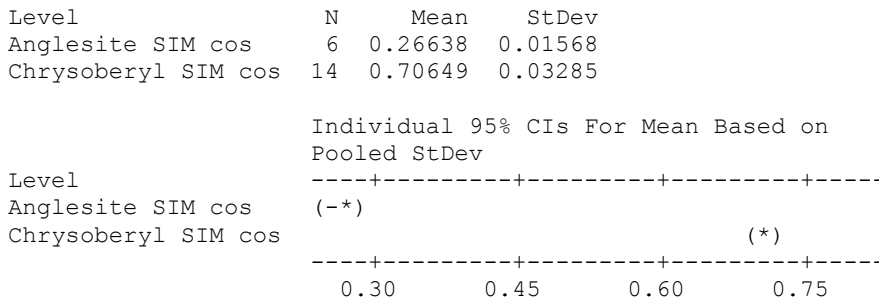


Pooled StDev = 0.1019

**One-way ANOVA: Anglesite SIM cos, Chrysoberyl SIM cos**

Source	DF	SS	MS	F	P
Factor	1	0.813525	0.813525	959.61	0.000
Error	18	0.015260	0.000848		
Total	19	0.828785			

S = 0.02912 R-Sq = 98.16% R-Sq(adj) = 98.06%



Pooled StDev = 0.02912

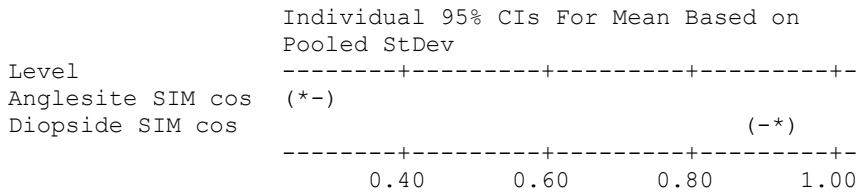
**One-way ANOVA: Anglesite SIM cos, Diopside SIM cos**

Source	DF	SS	MS	F	P
Factor	1	1.55505	1.55505	1328.45	0.000
Error	14	0.01639	0.00117		
Total	15	1.57144			

S = 0.03421 R-Sq = 98.96% R-Sq(adj) = 98.88%

Level	N	Mean	StDev
Anglesite SIM cos	6	0.26638	0.01568

Diopside SIM cos 10 0.91034 0.04104



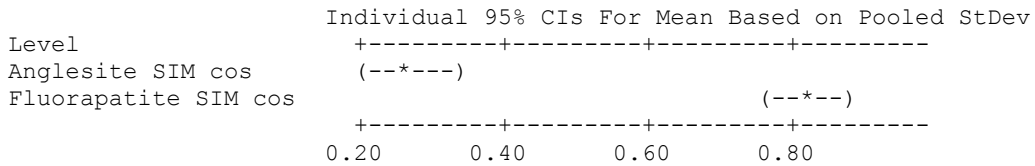
Pooled StDev = 0.03421

**One-way ANOVA: Anglesite SIM cos, Fluorapatite SIM cos**

Source	DF	SS	MS	F	P
Factor	1	0.90772	0.90772	175.75	0.000
Error	10	0.05165	0.00516		
Total	11	0.95937			

S = 0.07187 R-Sq = 94.62% R-Sq(adj) = 94.08%

Level	N	Mean	StDev
Anglesite SIM cos	6	0.26638	0.01568
Fluorapatite SIM cos	6	0.81645	0.10042

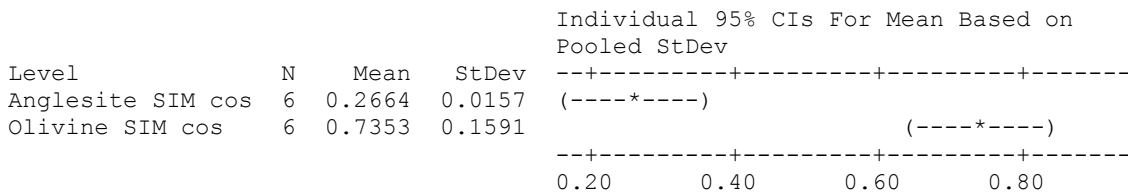


Pooled StDev = 0.07187

**One-way ANOVA: Anglesite SIM cos, Olivine SIM cos**

Source	DF	SS	MS	F	P
Factor	1	0.6597	0.6597	51.62	0.000
Error	10	0.1278	0.0128		
Total	11	0.7876			

S = 0.1131 R-Sq = 83.77% R-Sq(adj) = 82.15%



Pooled StDev = 0.1131

**One-way ANOVA: Anglesite SIM cos, Sapphire SIM cos**

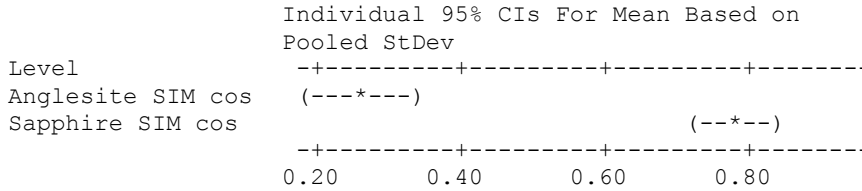
Source	DF	SS	MS	F	P
Factor	1	0.90636	0.90636	118.78	0.000
Error	12	0.09156	0.00763		



Total 13 0.99792

S = 0.08735 R-Sq = 90.82% R-Sq(adj) = 90.06%

Level	N	Mean	StDev
Anglesite SIM cos	6	0.26638	0.01568
Sapphire SIM cos	8	0.78054	0.11360



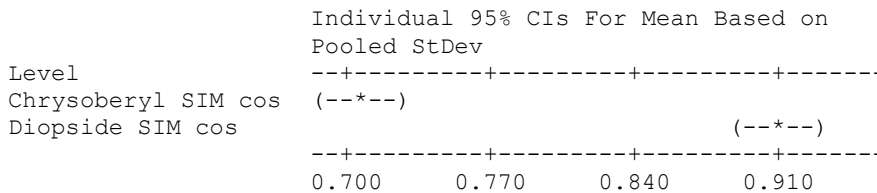
Pooled StDev = 0.08735

### One-way ANOVA: Chrysoberyl SIM cos, Diopside SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.24240	0.24240	182.70	0.000
Error	22	0.02919	0.00133		
Total	23	0.27158			

S = 0.03642 R-Sq = 89.25% R-Sq(adj) = 88.76%

Level	N	Mean	StDev
Chrysoberyl SIM cos	14	0.70649	0.03285
Diopside SIM cos	10	0.91034	0.04104



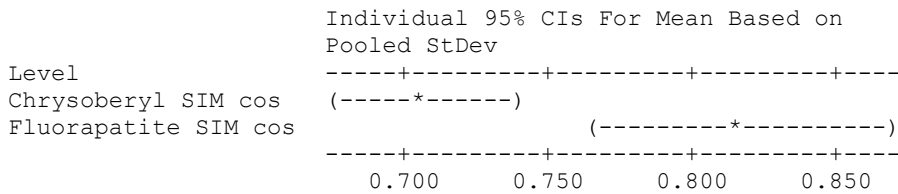
Pooled StDev = 0.03642

### One-way ANOVA: Chrysoberyl SIM cos, Fluorapatite SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.05078	0.05078	14.18	0.001
Error	18	0.06445	0.00358		
Total	19	0.11523			

S = 0.05984 R-Sq = 44.07% R-Sq(adj) = 40.96%

Level	N	Mean	StDev
Chrysoberyl SIM cos	14	0.70649	0.03285
Fluorapatite SIM cos	6	0.81645	0.10042



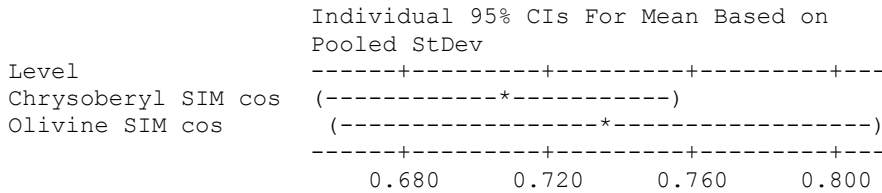
Pooled StDev = 0.05984

### One-way ANOVA: Chrysoberyl SIM cos, Olivine SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.00349	0.00349	0.45	0.512
Error	18	0.14061	0.00781		
Total	19	0.14410			

S = 0.08838 R-Sq = 2.42% R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Chrysoberyl SIM cos	14	0.70649	0.03285
Olivine SIM cos	6	0.73533	0.15911



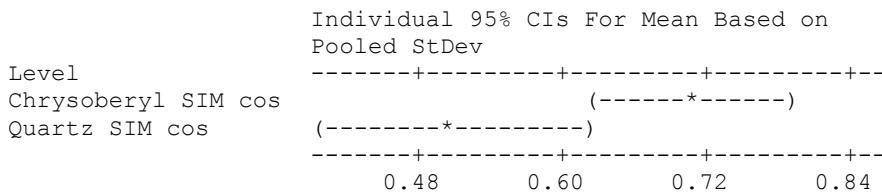
Pooled StDev = 0.08838

### One-way ANOVA: Chrysoberyl SIM cos, Quartz SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.1803	0.1803	7.94	0.011
Error	19	0.4316	0.0227		
Total	20	0.6120			

S = 0.1507 R-Sq = 29.47% R-Sq(adj) = 25.76%

Level	N	Mean	StDev
Chrysoberyl SIM cos	14	0.7065	0.0329
Quartz SIM cos	7	0.5099	0.2638



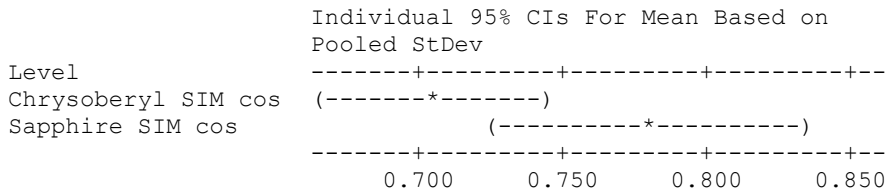
Pooled StDev = 0.1507

### One-way ANOVA: Chrysoberyl SIM cos, Sapphire SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.02791	0.02791	5.35	0.032
Error	20	0.10436	0.00522		
Total	21	0.13228			

S = 0.07224    R-Sq = 21.10%    R-Sq(adj) = 17.16%

Level	N	Mean	StDev
Chrysoberyl SIM cos	14	0.70649	0.03285
Sapphire SIM cos	8	0.78054	0.11360



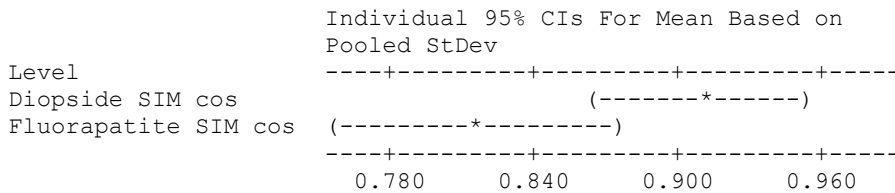
Pooled StDev = 0.07224

### One-way ANOVA: Diopside SIM cos, Fluorapatite SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.03306	0.03306	7.06	0.019
Error	14	0.06558	0.00468		
Total	15	0.09864			

S = 0.06844    R-Sq = 33.51%    R-Sq(adj) = 28.77%

Level	N	Mean	StDev
Diopside SIM cos	10	0.91034	0.04104
Fluorapatite SIM cos	6	0.81645	0.10042

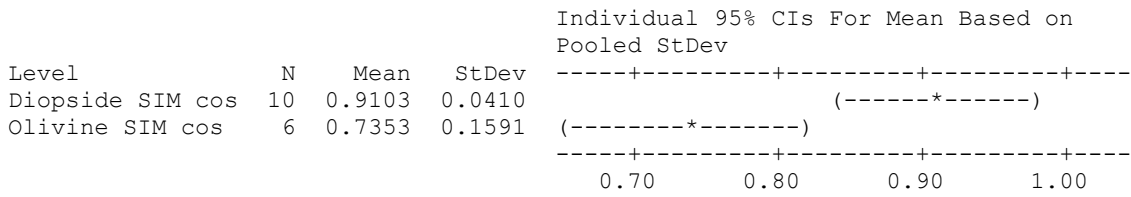


Pooled StDev = 0.06844

### One-way ANOVA: Diopside SIM cos, Olivine SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.1149	0.1149	11.34	0.005
Error	14	0.1417	0.0101		
Total	15	0.2566			

S = 0.1006    R-Sq = 44.76%    R-Sq(adj) = 40.82%

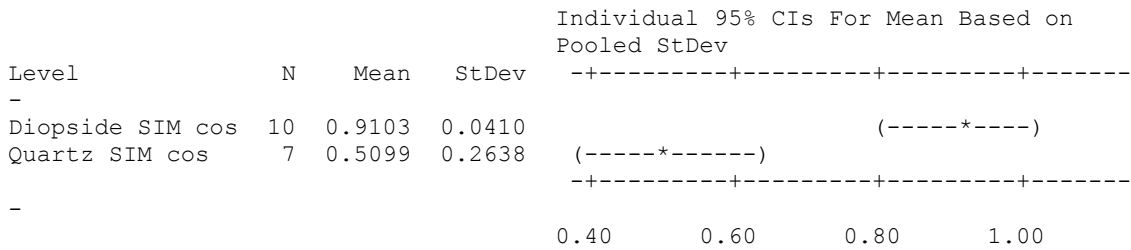


Pooled StDev = 0.1006

### One-way ANOVA: Diopside SIM cos, Quartz SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.6602	0.6602	22.88	0.000
Error	15	0.4328	0.0289		
Total	16	1.0930			

S = 0.1699 R-Sq = 60.41% R-Sq(adj) = 57.77%

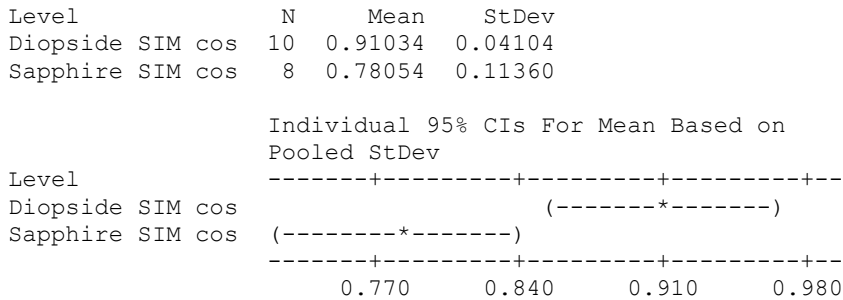


Pooled StDev = 0.1699

### One-way ANOVA: Diopside SIM cos, Sapphire SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.07488	0.07488	11.36	0.004
Error	16	0.10549	0.00659		
Total	17	0.18038			

S = 0.08120 R-Sq = 41.52% R-Sq(adj) = 37.86%



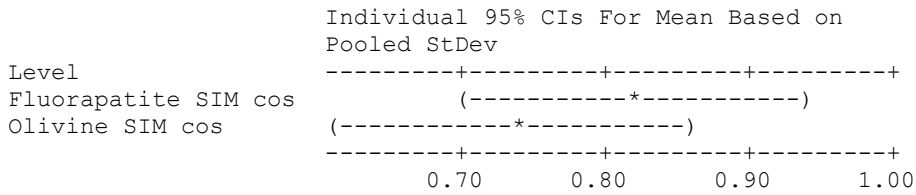
Pooled StDev = 0.08120

### One-way ANOVA: Fluorapatite SIM cos, Olivine SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.0197	0.0197	1.12	0.316
Error	10	0.1770	0.0177		
Total	11	0.1967			

S = 0.1330    R-Sq = 10.03%    R-Sq(adj) = 1.04%

Level	N	Mean	StDev
Fluorapatite SIM cos	6	0.8165	0.1004
Olivine SIM cos	6	0.7353	0.1591



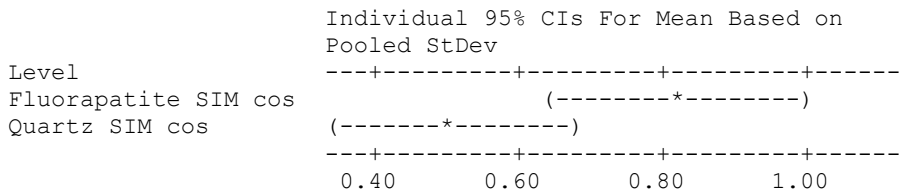
Pooled StDev = 0.1330

### One-way ANOVA: Fluorapatite SIM cos, Quartz SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.3036	0.3036	7.13	0.022
Error	11	0.4680	0.0425		
Total	12	0.7716			

S = 0.2063    R-Sq = 39.34%    R-Sq(adj) = 33.83%

Level	N	Mean	StDev
Fluorapatite SIM cos	6	0.8165	0.1004
Quartz SIM cos	7	0.5099	0.2638



Pooled StDev = 0.2063

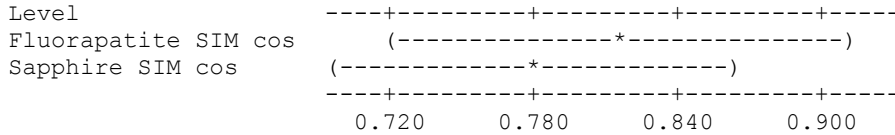
### One-way ANOVA: Fluorapatite SIM cos, Sapphire SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.0044	0.0044	0.38	0.551
Error	12	0.1408	0.0117		
Total	13	0.1452			

S = 0.1083    R-Sq = 3.05%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Fluorapatite SIM cos	6	0.8165	0.1004
Sapphire SIM cos	8	0.7805	0.1136

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.1083

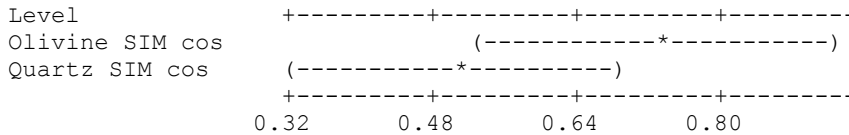
### One-way ANOVA: Olivine SIM cos, Quartz SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.1642	0.1642	3.32	0.096
Error	11	0.5442	0.0495		
Total	12	0.7084			

S = 0.2224 R-Sq = 23.18% R-Sq(adj) = 16.19%

Level	N	Mean	StDev
Olivine SIM cos	6	0.7353	0.1591
Quartz SIM cos	7	0.5099	0.2638

Individual 95% CIs For Mean Based on Pooled StDev



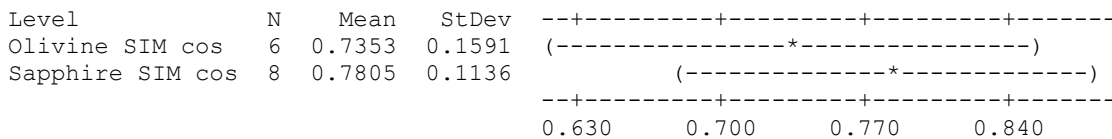
Pooled StDev = 0.2224

### One-way ANOVA: Olivine SIM cos, Sapphire SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.0070	0.0070	0.39	0.545
Error	12	0.2169	0.0181		
Total	13	0.2239			

S = 0.1344 R-Sq = 3.13% R-Sq(adj) = 0.00%

Individual 95% CIs For Mean Based on Pooled StDev

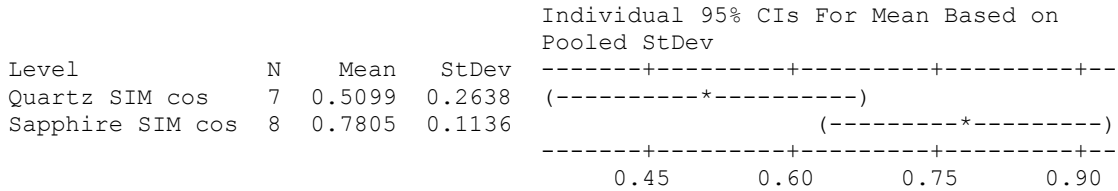


Pooled StDev = 0.1344

### One-way ANOVA: Quartz SIM cos, Sapphire SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.2734	0.2734	7.00	0.020
Error	13	0.5079	0.0391		
Total	14	0.7814			

S = 0.1977    R-Sq = 34.99%    R-Sq(adj) = 29.99%

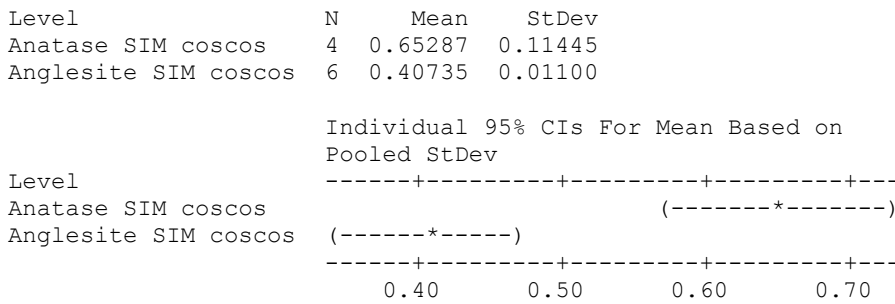


Pooled StDev = 0.1977

### One-way ANOVA: Anatase SIM coscos, Anglesite SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.14468	0.14468	29.01	0.001
Error	8	0.03990	0.00499		
Total	9	0.18458			

S = 0.07062    R-Sq = 78.38%    R-Sq(adj) = 75.68%



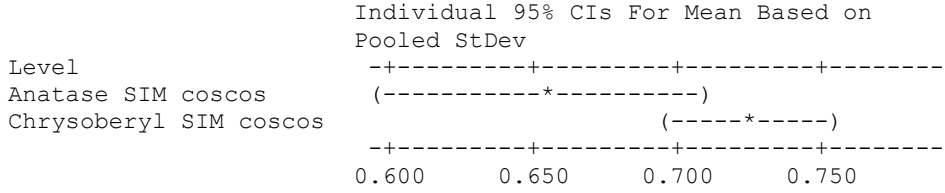
Pooled StDev = 0.07062

### One-way ANOVA: Anatase SIM coscos, Chrysoberyl SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.01689	0.01689	5.71	0.030
Error	16	0.04736	0.00296		
Total	17	0.06426			

S = 0.05441    R-Sq = 26.29%    R-Sq(adj) = 21.68%

Level	N	Mean	StDev
Anatase SIM coscos	4	0.65287	0.11445
Chrysoberyl SIM coscos	14	0.72656	0.02491



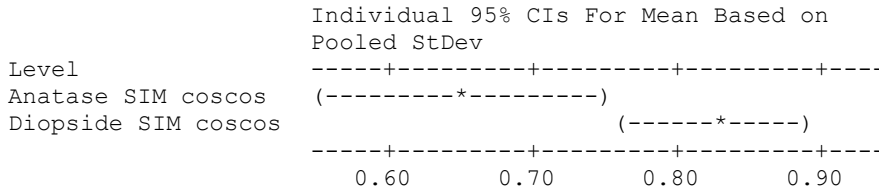
Pooled StDev = 0.05441

### One-way ANOVA: Anatase SIM coscos, Diopside SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.08701	0.08701	9.95	0.008
Error	12	0.10490	0.00874		
Total	13	0.19191			

S = 0.09350 R-Sq = 45.34% R-Sq(adj) = 40.78%

Level	N	Mean	StDev
Anatase SIM coscos	4	0.65287	0.11445
Diopside SIM coscos	10	0.82738	0.08538



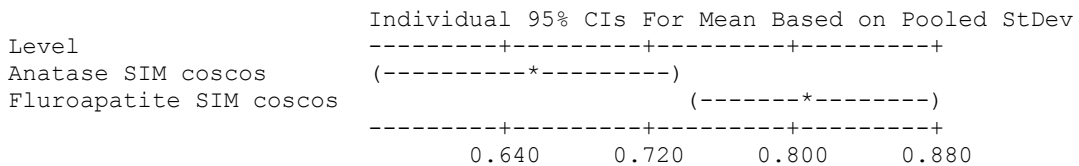
Pooled StDev = 0.09350

### One-way ANOVA: Anatase SIM coscos, Fluroapatite SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.05992	0.05992	11.72	0.009
Error	8	0.04091	0.00511		
Total	9	0.10083			

S = 0.07151 R-Sq = 59.43% R-Sq(adj) = 54.35%

Level	N	Mean	StDev
Anatase SIM coscos	4	0.65287	0.11445
Fluroapatite SIM coscos	6	0.81088	0.01798



Pooled StDev = 0.07151

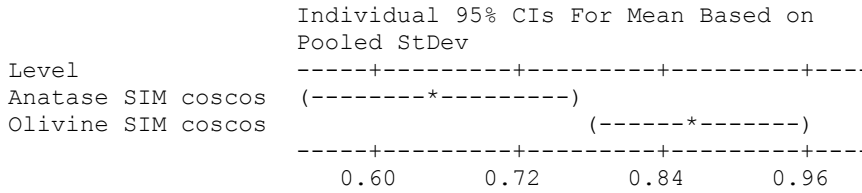


### One-way ANOVA: Anatase SIM coscos, Olivine SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.11100	0.11100	11.48	0.010
Error	8	0.07738	0.00967		
Total	9	0.18838			

S = 0.09835    R-Sq = 58.92%    R-Sq(adj) = 53.79%

Level	N	Mean	StDev
Anatase SIM coscos	4	0.65287	0.11445
Olivine SIM coscos	6	0.86793	0.08728

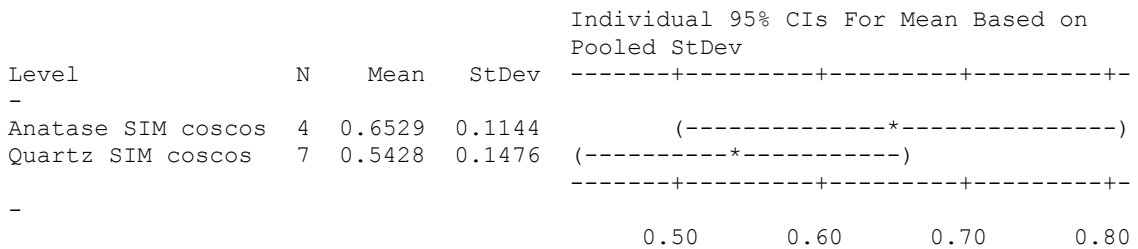


Pooled StDev = 0.09835

### One-way ANOVA: Anatase SIM coscos, Quartz SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.0309	0.0309	1.63	0.233
Error	9	0.1700	0.0189		
Total	10	0.2009			

S = 0.1374    R-Sq = 15.36%    R-Sq(adj) = 5.96%



Pooled StDev = 0.1374

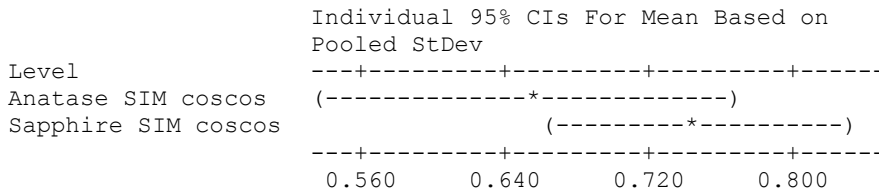
### One-way ANOVA: Anatase SIM coscos, Sapphire SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.0225	0.0225	2.02	0.186
Error	10	0.1117	0.0112		
Total	11	0.1343			

S = 0.1057    R-Sq = 16.79%    R-Sq(adj) = 8.47%

Level	N	Mean	StDev
Anatase SIM coscos	4	0.6529	0.1144

Sapphire SIM coscos 8 0.7448 0.1017



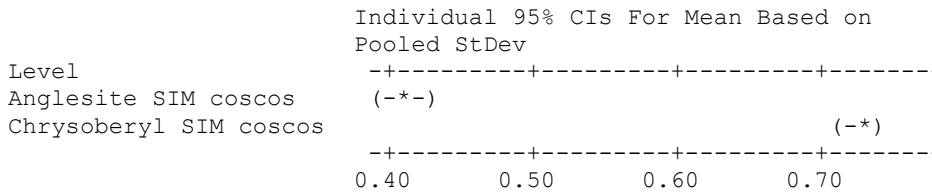
Pooled StDev = 0.1057

### One-way ANOVA: Anglesite SIM coscos, Chrysoberyl SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.427971	0.427971	888.05	0.000
Error	18	0.008675	0.000482		
Total	19	0.436645			

S = 0.02195 R-Sq = 98.01% R-Sq(adj) = 97.90%

Level	N	Mean	StDev
Anglesite SIM coscos	6	0.40735	0.01100
Chrysoberyl SIM coscos	14	0.72656	0.02491



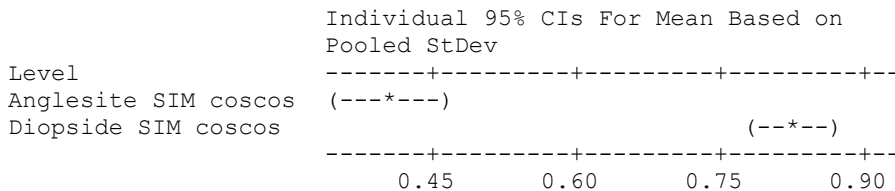
Pooled StDev = 0.02195

### One-way ANOVA: Anglesite SIM coscos, Diopside SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.66159	0.66159	139.89	0.000
Error	14	0.06621	0.00473		
Total	15	0.72781			

S = 0.06877 R-Sq = 90.90% R-Sq(adj) = 90.25%

Level	N	Mean	StDev
Anglesite SIM coscos	6	0.40735	0.01100
Diopside SIM coscos	10	0.82738	0.08538



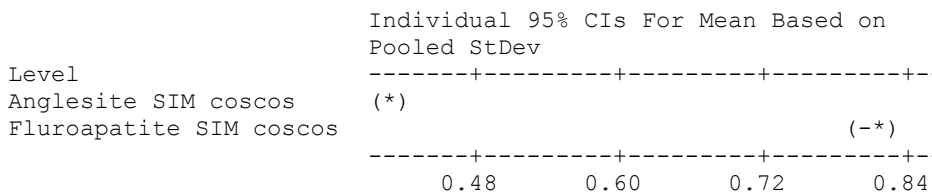
Pooled StDev = 0.06877

**One-way ANOVA: Anglesite SIM coscos, Fluroapatite SIM coscos**

Source	DF	SS	MS	F	P
Factor	1	0.488517	0.488517	2199.50	0.000
Error	10	0.002221	0.000222		
Total	11	0.490738			

S = 0.01490 R-Sq = 99.55% R-Sq(adj) = 99.50%

Level	N	Mean	StDev
Anglesite SIM coscos	6	0.40735	0.01100
Fluroapatite SIM coscos	6	0.81088	0.01798



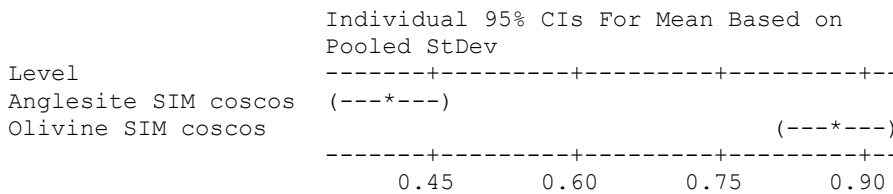
Pooled StDev = 0.01490

**One-way ANOVA: Anglesite SIM coscos, Olivine SIM coscos**

Source	DF	SS	MS	F	P
Factor	1	0.63641	0.63641	164.48	0.000
Error	10	0.03869	0.00387		
Total	11	0.67510			

S = 0.06220 R-Sq = 94.27% R-Sq(adj) = 93.70%

Level	N	Mean	StDev
Anglesite SIM coscos	6	0.40735	0.01100
Olivine SIM coscos	6	0.86793	0.08728



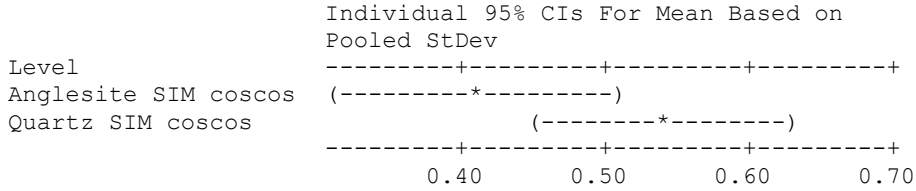
Pooled StDev = 0.06220

**One-way ANOVA: Anglesite SIM coscos, Quartz SIM coscos**

Source	DF	SS	MS	F	P
Factor	1	0.0592	0.0592	4.96	0.048
Error	11	0.1313	0.0119		
Total	12	0.1906			

S = 0.1093 R-Sq = 31.09% R-Sq(adj) = 24.83%

Level	N	Mean	StDev
Anglesite SIM coscos	6	0.4073	0.0110
Quartz SIM coscos	7	0.5428	0.1476



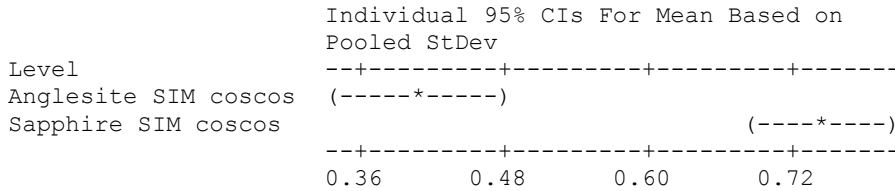
Pooled StDev = 0.1093

### One-way ANOVA: Anglesite SIM coscos, Sapphire SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.39048	0.39048	64.14	0.000
Error	12	0.07305	0.00609		
Total	13	0.46353			

S = 0.07802    R-Sq = 84.24%    R-Sq(adj) = 82.93%

Level	N	Mean	StDev
Anglesite SIM coscos	6	0.40735	0.01100
Sapphire SIM coscos	8	0.74483	0.10173



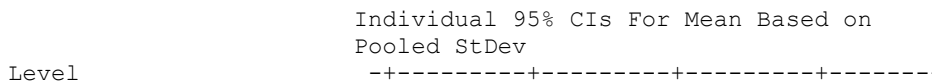
Pooled StDev = 0.07802

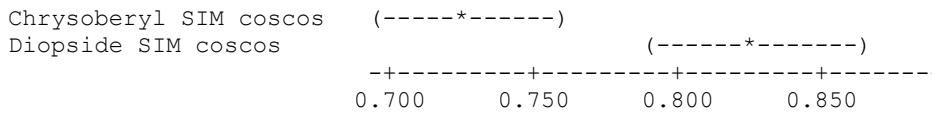
### One-way ANOVA: Chrysoberyl SIM coscos, Diopside SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.05929	0.05929	17.70	0.000
Error	22	0.07367	0.00335		
Total	23	0.13296			

S = 0.05787    R-Sq = 44.59%    R-Sq(adj) = 42.07%

Level	N	Mean	StDev
Chrysoberyl SIM coscos	14	0.72656	0.02491
Diopside SIM coscos	10	0.82738	0.08538





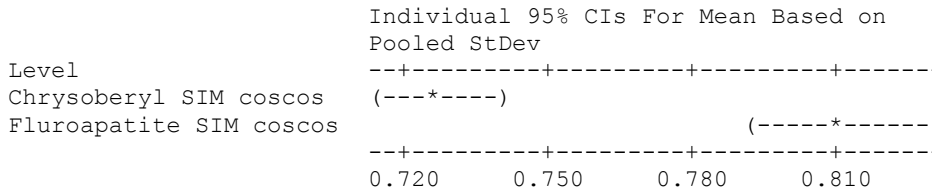
Pooled StDev = 0.05787

**One-way ANOVA: Chrysoberyl SIM coscos, Fluroapatite SIM coscos**

Source	DF	SS	MS	F	P
Factor	1	0.029861	0.029861	55.50	0.000
Error	18	0.009685	0.000538		
Total	19	0.039546			

S = 0.02320 R-Sq = 75.51% R-Sq(adj) = 74.15%

Level	N	Mean	StDev
Chrysoberyl SIM coscos	14	0.72656	0.02491
Fluroapatite SIM coscos	6	0.81088	0.01798



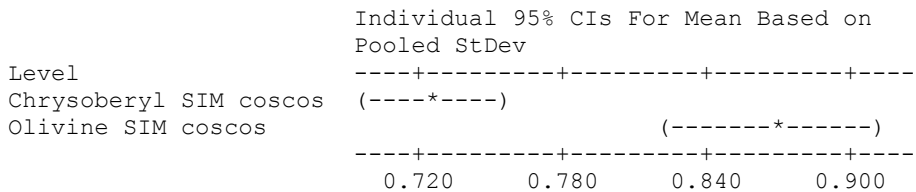
Pooled StDev = 0.02320

**One-way ANOVA: Chrysoberyl SIM coscos, Olivine SIM coscos**

Source	DF	SS	MS	F	P
Factor	1	0.08394	0.08394	32.73	0.000
Error	18	0.04616	0.00256		
Total	19	0.13009			

S = 0.05064 R-Sq = 64.52% R-Sq(adj) = 62.55%

Level	N	Mean	StDev
Chrysoberyl SIM coscos	14	0.72656	0.02491
Olivine SIM coscos	6	0.86793	0.08728



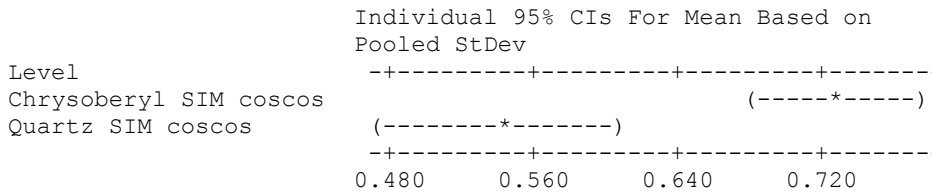
Pooled StDev = 0.05064

### One-way ANOVA: Chrysoberyl SIM coscos, Quartz SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.15764	0.15764	21.58	0.000
Error	19	0.13878	0.00730		
Total	20	0.29642			

S = 0.08547    R-Sq = 53.18%    R-Sq(adj) = 50.72%

Level	N	Mean	StDev
Chrysoberyl SIM coscos	14	0.72656	0.02491
Quartz SIM coscos	7	0.54277	0.14760



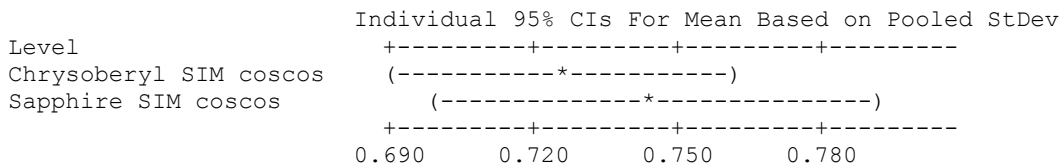
Pooled StDev = 0.08547

### One-way ANOVA: Chrysoberyl SIM coscos, Sapphire SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.00170	0.00170	0.42	0.523
Error	20	0.08052	0.00403		
Total	21	0.08221			

S = 0.06345    R-Sq = 2.06%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Chrysoberyl SIM coscos	14	0.72656	0.02491
Sapphire SIM coscos	8	0.74483	0.10173



Pooled StDev = 0.06345

### One-way ANOVA: Diopside SIM coscos, Fluroapatite SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.00102	0.00102	0.21	0.652
Error	14	0.06722	0.00480		
Total	15	0.06824			

S = 0.06929    R-Sq = 1.50%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Diopside SIM coscos	10	0.82738	0.08538
Fluroapatite SIM coscos	6	0.81088	0.01798

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Diopside SIM coscos	0.770	0.885
Fluroapatite SIM coscos	0.805	0.816

Pooled StDev = 0.06929

### One-way ANOVA: Diopside SIM coscos, Olivine SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.00617	0.00617	0.83	0.377
Error	14	0.10369	0.00741		
Total	15	0.10986			

S = 0.08606 R-Sq = 5.61% R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Diopside SIM coscos	10	0.82738	0.08538
Olivine SIM coscos	6	0.86793	0.08728

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Diopside SIM coscos	0.800	0.855
Olivine SIM coscos	0.850	0.885

Pooled StDev = 0.08606

### One-way ANOVA: Diopside SIM coscos, Quartz SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.3335	0.3335	25.48	0.000
Error	15	0.1963	0.0131		
Total	16	0.5299			

S = 0.1144 R-Sq = 62.95% R-Sq(adj) = 60.48%

Level	N	Mean	StDev
Diopside SIM coscos	10	0.8274	0.0854
Quartz SIM coscos	7	0.5428	0.1476

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Diopside SIM coscos	0.60	0.84
Quartz SIM coscos	0.48	0.60

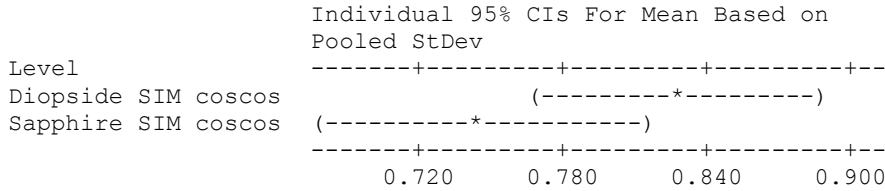
Pooled StDev = 0.1144

### One-way ANOVA: Diopside SIM coscos, Sapphire SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.03029	0.03029	3.51	0.079
Error	16	0.13805	0.00863		
Total	17	0.16834			

S = 0.09289 R-Sq = 17.99% R-Sq(adj) = 12.87%

Level	N	Mean	StDev
Diopside SIM coscos	10	0.82738	0.08538
Sapphire SIM coscos	8	0.74483	0.10173



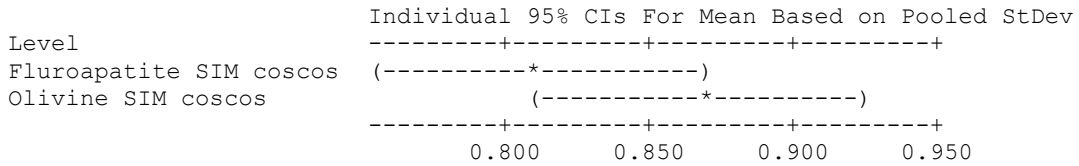
Pooled StDev = 0.09289

### One-way ANOVA: Fluroapatite SIM coscos, Olivine SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.00976	0.00976	2.46	0.148
Error	10	0.03970	0.00397		
Total	11	0.04947			

S = 0.06301 R-Sq = 19.74% R-Sq(adj) = 11.71%

Level	N	Mean	StDev
Fluroapatite SIM coscos	6	0.81088	0.01798
Olivine SIM coscos	6	0.86793	0.08728



Pooled StDev = 0.06301

### One-way ANOVA: Fluroapatite SIM coscos, Quartz SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.2322	0.2322	19.31	0.001
Error	11	0.1323	0.0120		
Total	12	0.3646			

S = 0.1097 R-Sq = 63.70% R-Sq(adj) = 60.40%



Level	N	Mean	StDev
Fluroapatite SIM coscos	6	0.8109	0.0180
Quartz SIM coscos	7	0.5428	0.1476

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower Bound	Upper Bound
Fluroapatite SIM coscos	0.7728	0.8490
Quartz SIM coscos	0.3952	0.7004

Pooled StDev = 0.1097

### One-way ANOVA: Fluroapatite SIM coscos, Sapphire SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.01496	0.01496	2.42	0.145
Error	12	0.07406	0.00617		
Total	13	0.08902			

S = 0.07856    R-Sq = 16.81%    R-Sq(adj) = 9.87%

Level	N	Mean	StDev
Fluroapatite SIM coscos	6	0.81088	0.01798
Sapphire SIM coscos	8	0.74483	0.10173

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower Bound	Upper Bound
Fluroapatite SIM coscos	0.7728	0.8490
Sapphire SIM coscos	0.6431	0.8466

Pooled StDev = 0.07856

### One-way ANOVA: Olivine SIM coscos, Quartz SIM coscos

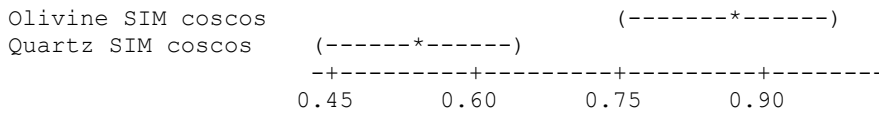
Source	DF	SS	MS	F	P
Factor	1	0.3416	0.3416	22.26	0.001
Error	11	0.1688	0.0153		
Total	12	0.5104			

S = 0.1239    R-Sq = 66.93%    R-Sq(adj) = 63.92%

Level	N	Mean	StDev
Olivine SIM coscos	6	0.8679	0.0873
Quartz SIM coscos	7	0.5428	0.1476

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower Bound	Upper Bound
Olivine SIM coscos	0.7806	0.9552
Quartz SIM coscos	0.3952	0.7004



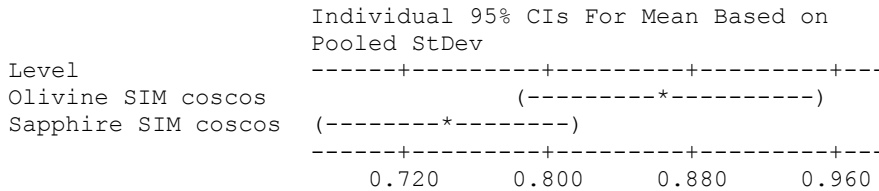
Pooled StDev = 0.1239

### One-way ANOVA: Olivine SIM coscos, Sapphire SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.05196	0.05196	5.64	0.035
Error	12	0.11053	0.00921		
Total	13	0.16250			

S = 0.09597 R-Sq = 31.98% R-Sq(adj) = 26.31%

Level	N	Mean	StDev
Olivine SIM coscos	6	0.86793	0.08728
Sapphire SIM coscos	8	0.74483	0.10173



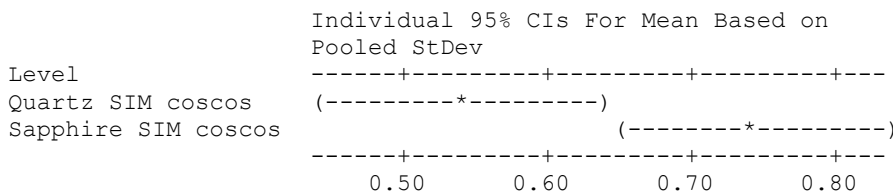
Pooled StDev = 0.09597

### One-way ANOVA: Quartz SIM coscos, Sapphire SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.1524	0.1524	9.75	0.008
Error	13	0.2032	0.0156		
Total	14	0.3556			

S = 0.1250 R-Sq = 42.86% R-Sq(adj) = 38.47%

Level	N	Mean	StDev
Quartz SIM coscos	7	0.5428	0.1476
Sapphire SIM coscos	8	0.7448	0.1017



Pooled StDev = 0.1250

### One-way ANOVA: Anatase SIM sincos, Anglesite SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.54253	0.54253	206.96	0.000

```
Error      8  0.02097  0.00262
Total     9  0.56350
```

S = 0.05120    R-Sq = 96.28%    R-Sq(adj) = 95.81%

```
Level              N      Mean      StDev
Anatase SIM sincos  4  0.73580  0.06707
Anglesite SIM sincos 6  0.26035  0.03867
```

Individual 95% CIs For Mean Based on Pooled StDev

```
Level
Anatase SIM sincos      (---*---)
Anglesite SIM sincos  (---*---)
-----+-----+-----+-----+-----+
                0.30      0.45      0.60      0.75
```

Pooled StDev = 0.05120

**One-way ANOVA: Anatase SIM sincos, Chrysoberyl SIM sincos**

```
Source  DF      SS      MS      F      P
Factor   1  0.02836  0.02836  16.78  0.001
Error   16  0.02704  0.00169
Total   17  0.05540
```

S = 0.04111    R-Sq = 51.19%    R-Sq(adj) = 48.14%

```
Level              N      Mean      StDev
Anatase SIM sincos  4  0.73580  0.06707
Chrysoberyl SIM sincos 14  0.83127  0.03228
```

Individual 95% CIs For Mean Based on Pooled StDev

```
Level
Anatase SIM sincos      (-----*-----)
Chrysoberyl SIM sincos      (---*---)
-----+-----+-----+-----+
                0.700      0.750      0.800      0.850
```

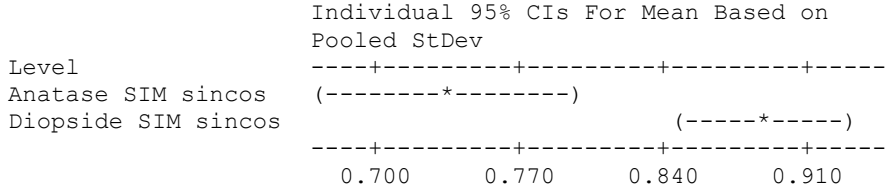
Pooled StDev = 0.04111

**One-way ANOVA: Anatase SIM sincos, Diopside SIM sincos**

```
Source  DF      SS      MS      F      P
Factor   1  0.06736  0.06736  19.83  0.001
Error   12  0.04075  0.00340
Total   13  0.10811
```

S = 0.05827    R-Sq = 62.31%    R-Sq(adj) = 59.16%

```
Level              N      Mean      StDev
Anatase SIM sincos  4  0.73580  0.06707
Diopside SIM sincos 10  0.88934  0.05503
```



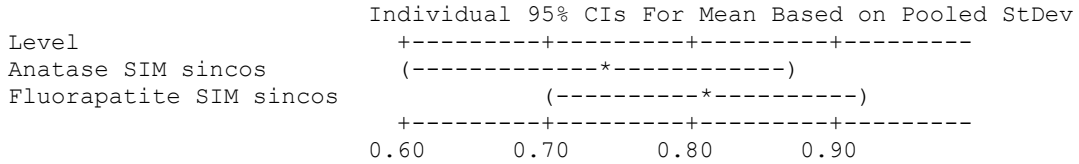
Pooled StDev = 0.05827

**One-way ANOVA: Anatase SIM sincos, Fluorapatite SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.0129	0.0129	0.91	0.368
Error	8	0.1128	0.0141		
Total	9	0.1257			

S = 0.1187    R-Sq = 10.23%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Anatase SIM sincos	4	0.7358	0.0671
Fluorapatite SIM sincos	6	0.8090	0.1409

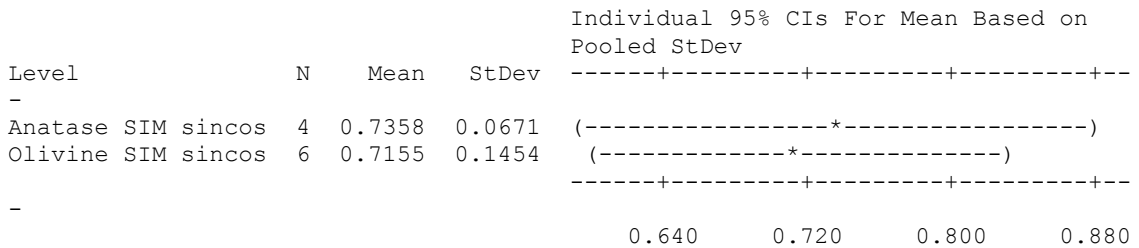


Pooled StDev = 0.1187

**One-way ANOVA: Anatase SIM sincos, Olivine SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.0010	0.0010	0.07	0.803
Error	8	0.1192	0.0149		
Total	9	0.1202			

S = 0.1221    R-Sq = 0.82%    R-Sq(adj) = 0.00%



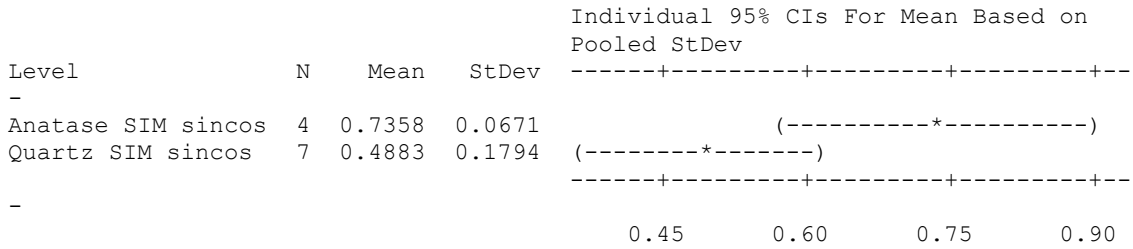
Pooled StDev = 0.1221

**One-way ANOVA: Anatase SIM sincos, Quartz SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.1559	0.1559	6.79	0.028

Error 9 0.2066 0.0230  
 Total 10 0.3625

S = 0.1515 R-Sq = 43.01% R-Sq(adj) = 36.68%



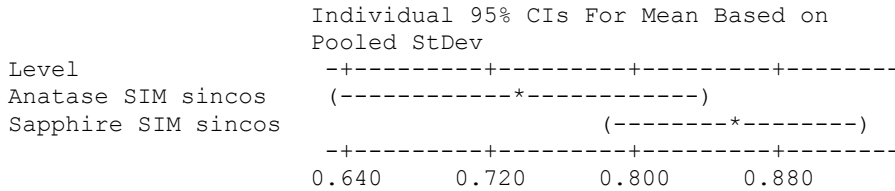
Pooled StDev = 0.1515

**One-way ANOVA: Anatase SIM sincos, Sapphire SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.03920	0.03920	4.83	0.053
Error	10	0.08120	0.00812		
Total	11	0.12039			

S = 0.09011 R-Sq = 32.56% R-Sq(adj) = 25.81%

Level	N	Mean	StDev
Anatase SIM sincos	4	0.73580	0.06707
Sapphire SIM sincos	8	0.85704	0.09834



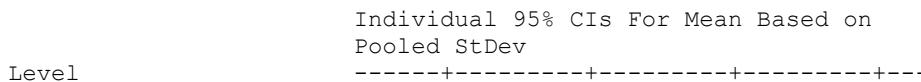
Pooled StDev = 0.09011

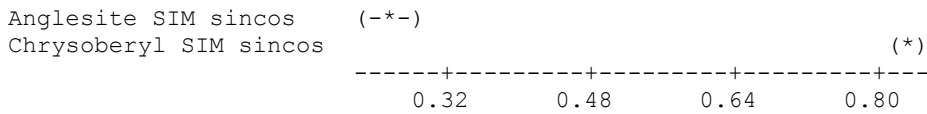
**One-way ANOVA: Anglesite SIM sincos, Chrysoberyl SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	1.36900	1.36900	1172.18	0.000
Error	18	0.02102	0.00117		
Total	19	1.39002			

S = 0.03417 R-Sq = 98.49% R-Sq(adj) = 98.40%

Level	N	Mean	StDev
Anglesite SIM sincos	6	0.26035	0.03867
Chrysoberyl SIM sincos	14	0.83127	0.03228





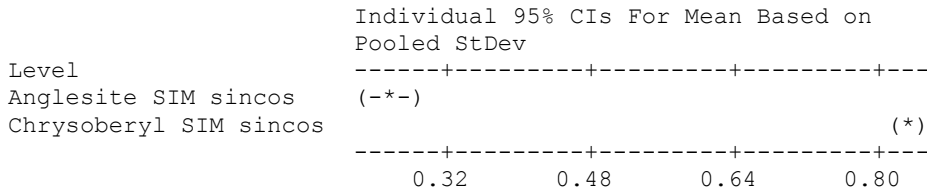
Pooled StDev = 0.03417

**One-way ANOVA: Anglesite SIM sincos, Chrysoberyl SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	1.36900	1.36900	1172.18	0.000
Error	18	0.02102	0.00117		
Total	19	1.39002			

S = 0.03417 R-Sq = 98.49% R-Sq(adj) = 98.40%

Level	N	Mean	StDev
Anglesite SIM sincos	6	0.26035	0.03867
Chrysoberyl SIM sincos	14	0.83127	0.03228



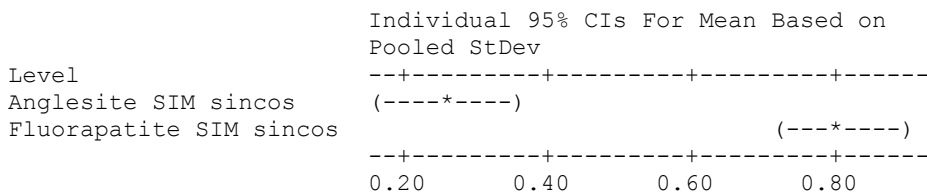
Pooled StDev = 0.03417

**One-way ANOVA: Anglesite SIM sincos, Fluorapatite SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.9031	0.9031	84.57	0.000
Error	10	0.1068	0.0107		
Total	11	1.0098			

S = 0.1033 R-Sq = 89.43% R-Sq(adj) = 88.37%

Level	N	Mean	StDev
Anglesite SIM sincos	6	0.2603	0.0387
Fluorapatite SIM sincos	6	0.8090	0.1409



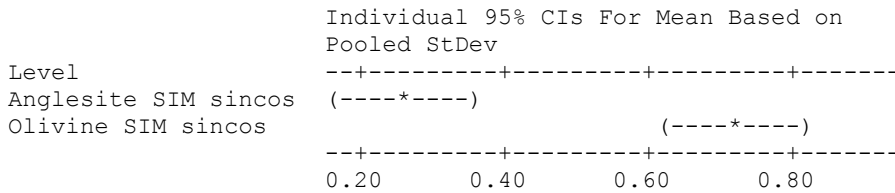
Pooled StDev = 0.1033

### One-way ANOVA: Anglesite SIM sincos, Olivine SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.6215	0.6215	54.92	0.000
Error	10	0.1132	0.0113		
Total	11	0.7347			

S = 0.1064    R-Sq = 84.60%    R-Sq(adj) = 83.06%

Level	N	Mean	StDev
Anglesite SIM sincos	6	0.2603	0.0387
Olivine SIM sincos	6	0.7155	0.1454



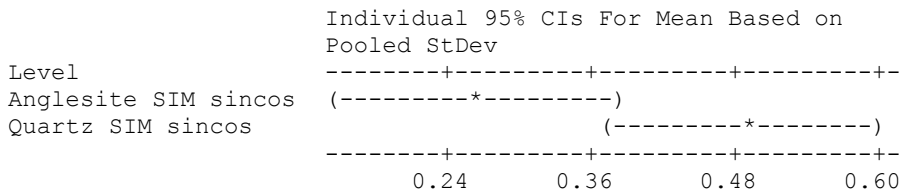
Pooled StDev = 0.1064

### One-way ANOVA: Anglesite SIM sincos, Quartz SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.1679	0.1679	9.21	0.011
Error	11	0.2005	0.0182		
Total	12	0.3684			

S = 0.1350    R-Sq = 45.57%    R-Sq(adj) = 40.62%

Level	N	Mean	StDev
Anglesite SIM sincos	6	0.2603	0.0387
Quartz SIM sincos	7	0.4883	0.1794



Pooled StDev = 0.1350

### One-way ANOVA: Anglesite SIM sincos, Sapphire SIM sincos

Source	DF	SS	MS	F	P
Factor	1	1.22069	1.22069	194.85	0.000
Error	12	0.07518	0.00626		
Total	13	1.29587			

S = 0.07915    R-Sq = 94.20%    R-Sq(adj) = 93.72%

Level	N	Mean	StDev
Anglesite SIM sincos	6	0.26035	0.03867
Sapphire SIM sincos	8	0.85704	0.09834

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anglesite SIM sincos	(---*---)
Sapphire SIM sincos	(--*--)

0.20      0.40      0.60      0.80

Pooled StDev = 0.07915

### One-way ANOVA: Chrysoberyl SIM sincos, Diopside SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.01967	0.01967	10.61	0.004
Error	22	0.04080	0.00185		
Total	23	0.06047			

S = 0.04307    R-Sq = 32.53%    R-Sq(adj) = 29.46%

Level	N	Mean	StDev
Chrysoberyl SIM sincos	14	0.83127	0.03228
Diopside SIM sincos	10	0.88934	0.05503

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Chrysoberyl SIM sincos	(-----*-----)
Diopside SIM sincos	(-----*-----)

0.810      0.840      0.870      0.900

Pooled StDev = 0.04307

### One-way ANOVA: Chrysoberyl SIM sincos, Diopside SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.01967	0.01967	10.61	0.004
Error	22	0.04080	0.00185		
Total	23	0.06047			

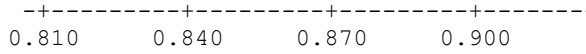
S = 0.04307    R-Sq = 32.53%    R-Sq(adj) = 29.46%

Level	N	Mean	StDev
Chrysoberyl SIM sincos	14	0.83127	0.03228
Diopside SIM sincos	10	0.88934	0.05503

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Chrysoberyl SIM sincos	(-----*-----)
Diopside SIM sincos	(-----*-----)





Pooled StDev = 0.04307

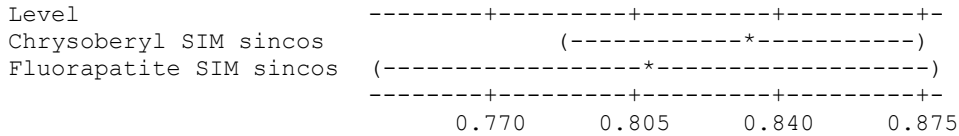
**One-way ANOVA: Chrysoberyl SIM sincos, Fluorapatite SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.00208	0.00208	0.33	0.571
Error	18	0.11284	0.00627		
Total	19	0.11493			

S = 0.07918    R-Sq = 1.81%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Chrysoberyl SIM sincos	14	0.83127	0.03228
Fluorapatite SIM sincos	6	0.80900	0.14092

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.07918

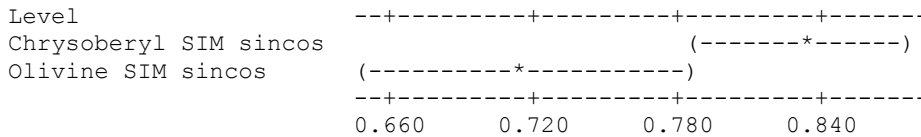
**One-way ANOVA: Chrysoberyl SIM sincos, Olivine SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.05628	0.05628	8.49	0.009
Error	18	0.11925	0.00662		
Total	19	0.17552			

S = 0.08139    R-Sq = 32.06%    R-Sq(adj) = 28.29%

Level	N	Mean	StDev
Chrysoberyl SIM sincos	14	0.83127	0.03228
Olivine SIM sincos	6	0.71552	0.14540

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.08139

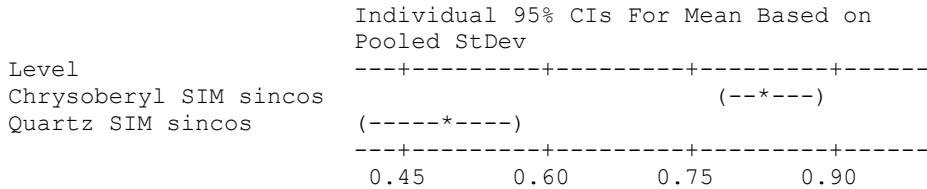
**One-way ANOVA: Chrysoberyl SIM sincos, Quartz SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.5489	0.5489	50.48	0.000

Error 19 0.2066 0.0109  
 Total 20 0.7555

S = 0.1043 R-Sq = 72.65% R-Sq(adj) = 71.21%

Level	N	Mean	StDev
Chrysoberyl SIM sincos	14	0.8313	0.0323
Quartz SIM sincos	7	0.4883	0.1794



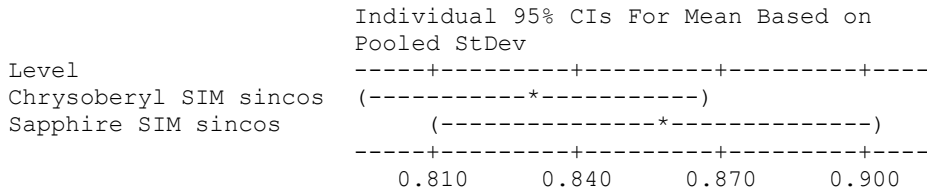
Pooled StDev = 0.1043

**One-way ANOVA: Chrysoberyl SIM sincos, Sapphire SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.00338	0.00338	0.83	0.373
Error	20	0.08125	0.00406		
Total	21	0.08463			

S = 0.06374 R-Sq = 3.99% R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Chrysoberyl SIM sincos	14	0.83127	0.03228
Sapphire SIM sincos	8	0.85704	0.09834



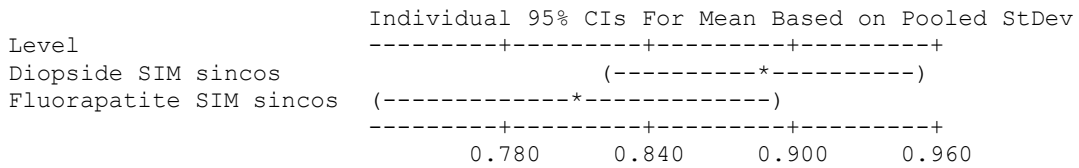
Pooled StDev = 0.06374

**One-way ANOVA: Diopside SIM sincos, Fluorapatite SIM sincos**

Source	DF	SS	MS	F	P
Factor	1	0.02420	0.02420	2.68	0.124
Error	14	0.12655	0.00904		
Total	15	0.15076			

S = 0.09508 R-Sq = 16.06% R-Sq(adj) = 10.06%

Level	N	Mean	StDev
Diopside SIM sincos	10	0.88934	0.05503
Fluorapatite SIM sincos	6	0.80900	0.14092



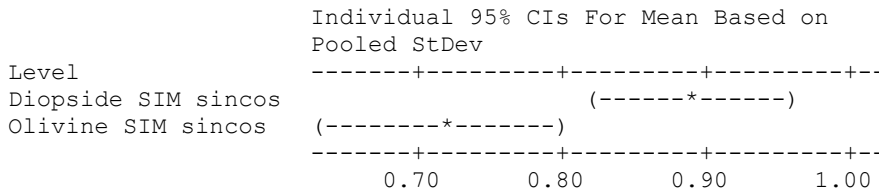
Pooled StDev = 0.09508

### One-way ANOVA: Diopside SIM sincos, Olivine SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.11330	0.11330	11.93	0.004
Error	14	0.13296	0.00950		
Total	15	0.24626			

S = 0.09745 R-Sq = 46.01% R-Sq(adj) = 42.15%

Level	N	Mean	StDev
Diopside SIM sincos	10	0.88934	0.05503
Olivine SIM sincos	6	0.71552	0.14540



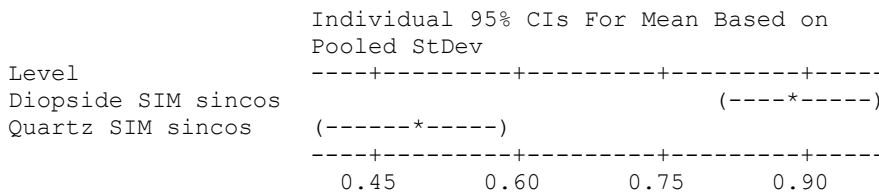
Pooled StDev = 0.09745

### One-way ANOVA: Diopside SIM sincos, Quartz SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.6622	0.6622	45.09	0.000
Error	15	0.2203	0.0147		
Total	16	0.8825			

S = 0.1212 R-Sq = 75.04% R-Sq(adj) = 73.37%

Level	N	Mean	StDev
Diopside SIM sincos	10	0.8893	0.0550
Quartz SIM sincos	7	0.4883	0.1794



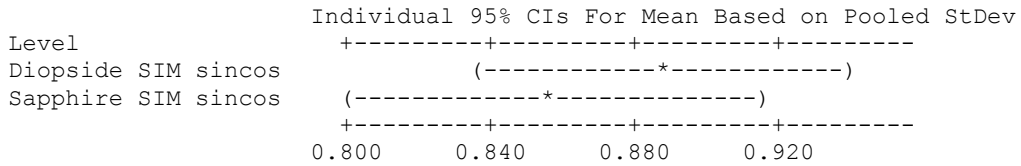
Pooled StDev = 0.1212

### One-way ANOVA: Diopside SIM sincos, Sapphire SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.00464	0.00464	0.78	0.390
Error	16	0.09496	0.00593		
Total	17	0.09959			

S = 0.07704    R-Sq = 4.66%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Diopside SIM sincos	10	0.88934	0.05503
Sapphire SIM sincos	8	0.85704	0.09834



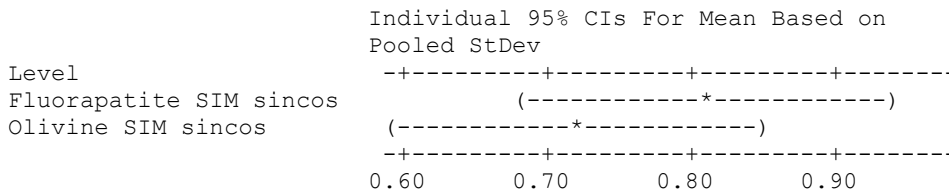
Pooled StDev = 0.07704

### One-way ANOVA: Fluorapatite SIM sincos, Olivine SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.0262	0.0262	1.28	0.284
Error	10	0.2050	0.0205		
Total	11	0.2312			

S = 0.1432    R-Sq = 11.34%    R-Sq(adj) = 2.47%

Level	N	Mean	StDev
Fluorapatite SIM sincos	6	0.8090	0.1409
Olivine SIM sincos	6	0.7155	0.1454



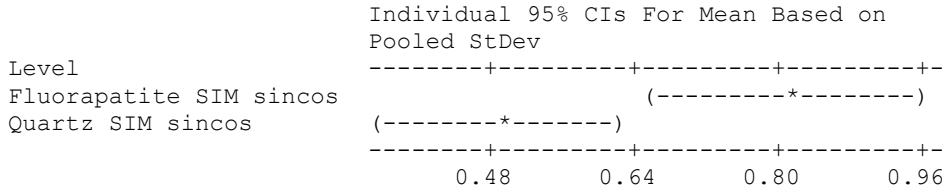
Pooled StDev = 0.1432

### One-way ANOVA: Fluorapatite SIM sincos, Quartz SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.3323	0.3323	12.50	0.005
Error	11	0.2924	0.0266		
Total	12	0.6246			

S = 0.1630    R-Sq = 53.19%    R-Sq(adj) = 48.94%

Level	N	Mean	StDev
Fluorapatite SIM sincos	6	0.8090	0.1409
Quartz SIM sincos	7	0.4883	0.1794



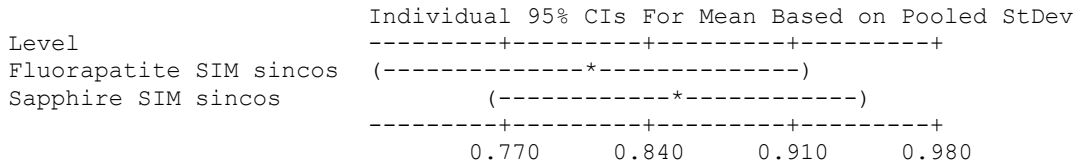
Pooled StDev = 0.1630

### One-way ANOVA: Fluorapatite SIM sincos, Sapphire SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.0079	0.0079	0.57	0.465
Error	12	0.1670	0.0139		
Total	13	0.1749			

S = 0.1180 R-Sq = 4.52% R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Fluorapatite SIM sincos	6	0.8090	0.1409
Sapphire SIM sincos	8	0.8570	0.0983

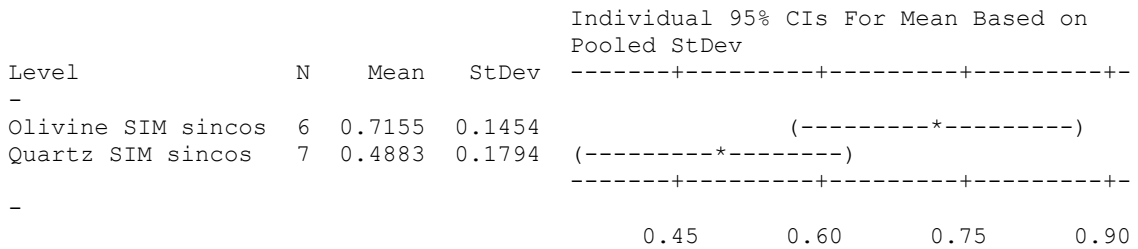


Pooled StDev = 0.1180

### One-way ANOVA: Olivine SIM sincos, Quartz SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.1668	0.1668	6.14	0.031
Error	11	0.2988	0.0272		
Total	12	0.4655			

S = 0.1648 R-Sq = 35.82% R-Sq(adj) = 29.99%



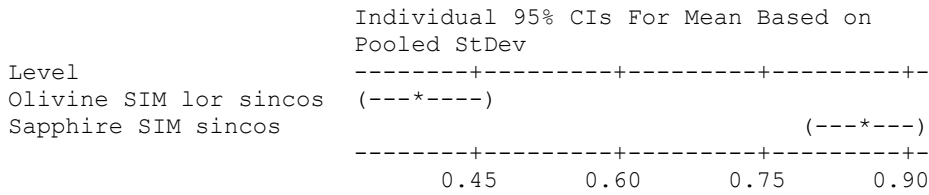
Pooled StDev = 0.1648

### One-way ANOVA: Olivine SIM lor sincos, Sapphire SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.74003	0.74003	130.78	0.000
Error	12	0.06790	0.00566		
Total	13	0.80793			

S = 0.07522    R-Sq = 91.60%    R-Sq(adj) = 90.90%

Level	N	Mean	StDev
Olivine SIM lor sincos	6	0.39245	0.00632
Sapphire SIM sincos	8	0.85704	0.09834



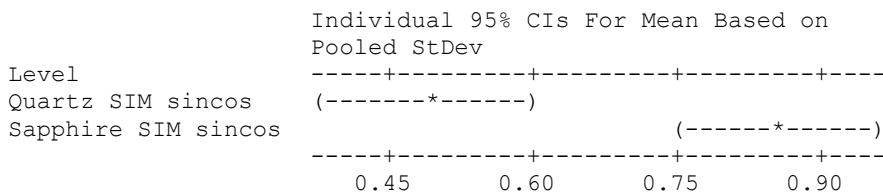
Pooled StDev = 0.07522

### One-way ANOVA: Quartz SIM sincos, Sapphire SIM sincos

Source	DF	SS	MS	F	P
Factor	1	0.5076	0.5076	25.30	0.000
Error	13	0.2608	0.0201		
Total	14	0.7683			

S = 0.1416    R-Sq = 66.06%    R-Sq(adj) = 63.45%

Level	N	Mean	StDev
Quartz SIM sincos	7	0.4883	0.1794
Sapphire SIM sincos	8	0.8570	0.0983



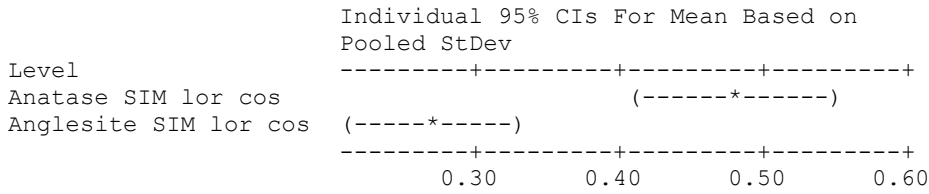
Pooled StDev = 0.1416

### One-way ANOVA: Anatase SIM lor cos, Anglesite SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.10914	0.10914	27.56	0.001
Error	8	0.03168	0.00396		
Total	9	0.14082			

S = 0.06293    R-Sq = 77.50%    R-Sq(adj) = 74.69%

Level	N	Mean	StDev
Anatase SIM lor cos	4	0.48100	0.10255
Anglesite SIM lor cos	6	0.26775	0.00518



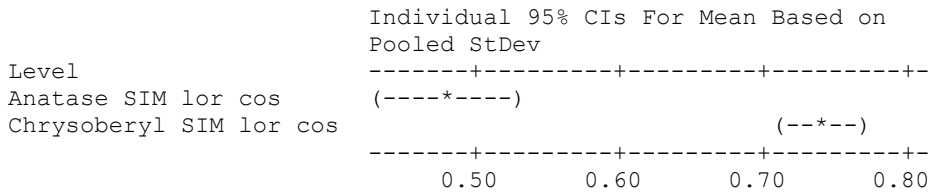
Pooled StDev = 0.06293

### One-way ANOVA: Anatase SIM lor cos, Chrysoberyl SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.21018	0.21018	87.87	0.000
Error	16	0.03827	0.00239		
Total	17	0.24846			

S = 0.04891    R-Sq = 84.60%    R-Sq(adj) = 83.63%

Level	N	Mean	StDev
Anatase SIM lor cos	4	0.48100	0.10255
Chrysoberyl SIM lor cos	14	0.74092	0.02275



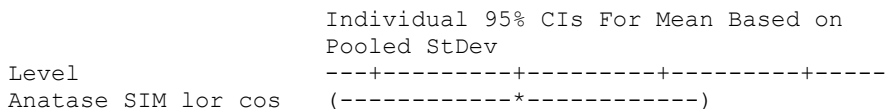
Pooled StDev = 0.04891

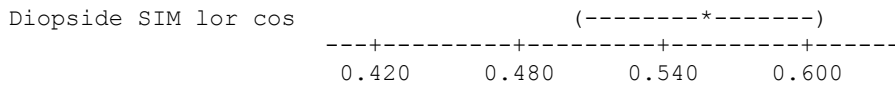
### One-way ANOVA: Anatase SIM lor cos, Diopside SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.01616	0.01616	3.13	0.102
Error	12	0.06202	0.00517		
Total	13	0.07818			

S = 0.07189    R-Sq = 20.67%    R-Sq(adj) = 14.06%

Level	N	Mean	StDev
Anatase SIM lor cos	4	0.48100	0.10255
Diopside SIM lor cos	10	0.55621	0.05819





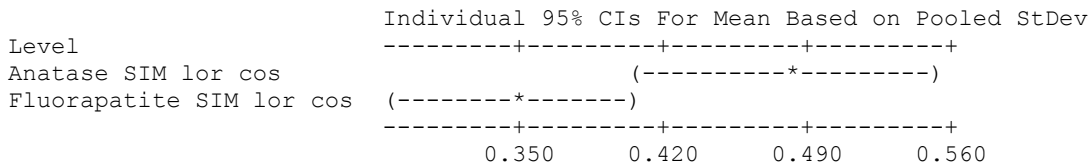
Pooled StDev = 0.07189

**One-way ANOVA: Anatase SIM lor cos, Fluorapatite SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.04260	0.04260	10.68	0.011
Error	8	0.03191	0.00399		
Total	9	0.07451			

S = 0.06316 R-Sq = 57.17% R-Sq(adj) = 51.82%

Level	N	Mean	StDev
Anatase SIM lor cos	4	0.48100	0.10255
Fluorapatite SIM lor cos	6	0.34777	0.00853



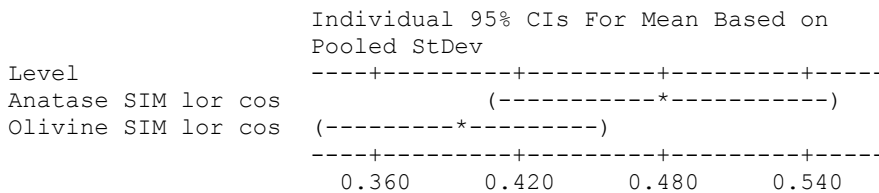
Pooled StDev = 0.06316

**One-way ANOVA: Anatase SIM lor cos, Olivine SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.01725	0.01725	4.25	0.073
Error	8	0.03245	0.00406		
Total	9	0.04970			

S = 0.06369 R-Sq = 34.71% R-Sq(adj) = 26.55%

Level	N	Mean	StDev
Anatase SIM lor cos	4	0.48100	0.10255
Olivine SIM lor cos	6	0.39622	0.01346



Pooled StDev = 0.06369

**One-way ANOVA: Anatase SIM lor cos, Quartz SIM lor cos**

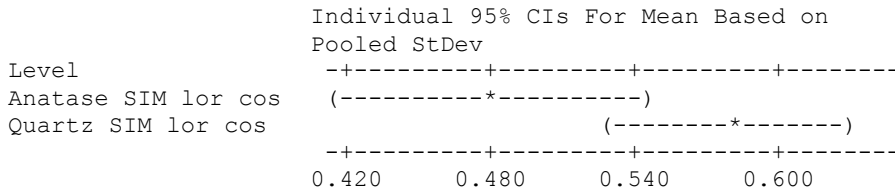
Source	DF	SS	MS	F	P
Factor	1	0.02540	0.02540	7.23	0.025
Error	9	0.03161	0.00351		



Total 10 0.05702

S = 0.05927 R-Sq = 44.55% R-Sq(adj) = 38.39%

Level	N	Mean	StDev
Anatase SIM lor cos	4	0.48100	0.10255
Quartz SIM lor cos	7	0.58090	0.00332



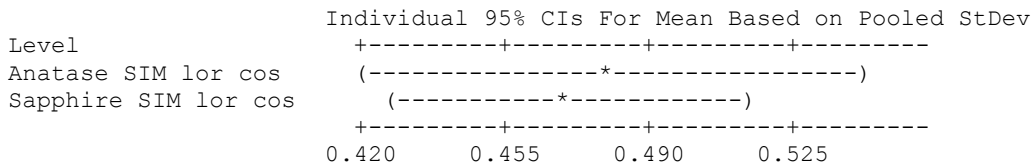
Pooled StDev = 0.05927

### One-way ANOVA: Anatase SIM lor cos, Sapphire SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.00034	0.00034	0.11	0.749
Error	10	0.03172	0.00317		
Total	11	0.03207			

S = 0.05632 R-Sq = 1.07% R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Anatase SIM lor cos	4	0.48100	0.10255
Sapphire SIM lor cos	8	0.46965	0.00504



Pooled StDev = 0.05632

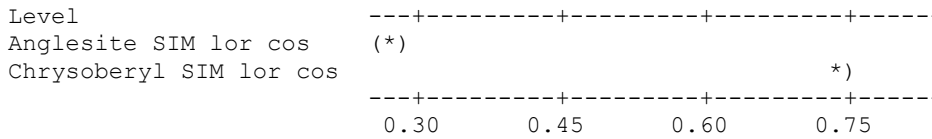
### One-way ANOVA: Anglesite SIM lor cos, Chrysoberyl SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.940343	0.940343	2467.46	0.000
Error	18	0.006860	0.000381		
Total	19	0.947203			

S = 0.01952 R-Sq = 99.28% R-Sq(adj) = 99.24%

Level	N	Mean	StDev
Anglesite SIM lor cos	6	0.26775	0.00518
Chrysoberyl SIM lor cos	14	0.74092	0.02275

Individual 95% CIs For Mean Based on Pooled StDev



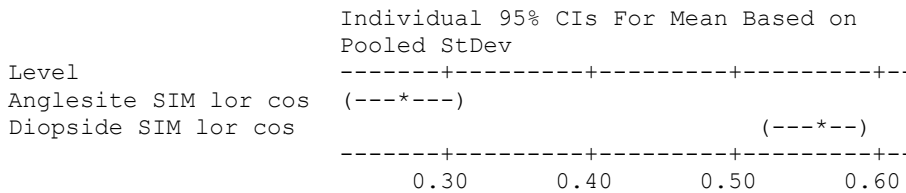
Pooled StDev = 0.01952

### One-way ANOVA: Anglesite SIM lor cos, Diopside SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.31203	0.31203	142.74	0.000
Error	14	0.03060	0.00219		
Total	15	0.34264			

S = 0.04676 R-Sq = 91.07% R-Sq(adj) = 90.43%

Level	N	Mean	StDev
Anglesite SIM lor cos	6	0.26775	0.00518
Diopside SIM lor cos	10	0.55621	0.05819



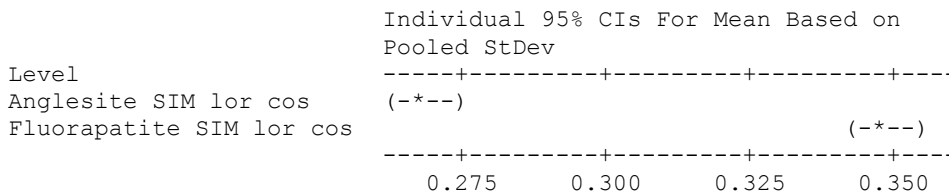
Pooled StDev = 0.04676

### One-way ANOVA: Anglesite SIM lor cos, Fluorapatite SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.0192080	0.0192080	385.82	0.000
Error	10	0.0004978	0.0000498		
Total	11	0.0197058			

S = 0.007056 R-Sq = 97.47% R-Sq(adj) = 97.22%

Level	N	Mean	StDev
Anglesite SIM lor cos	6	0.26775	0.00518
Fluorapatite SIM lor cos	6	0.34777	0.00853



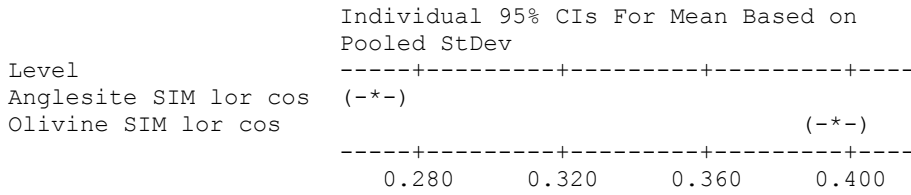
Pooled StDev = 0.00706

### One-way ANOVA: Anglesite SIM lor cos, Olivine SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.049511	0.049511	476.22	0.000
Error	10	0.001040	0.000104		
Total	11	0.050551			

S = 0.01020    R-Sq = 97.94%    R-Sq(adj) = 97.74%

Level	N	Mean	StDev
Anglesite SIM lor cos	6	0.26775	0.00518
Olivine SIM lor cos	6	0.39622	0.01346



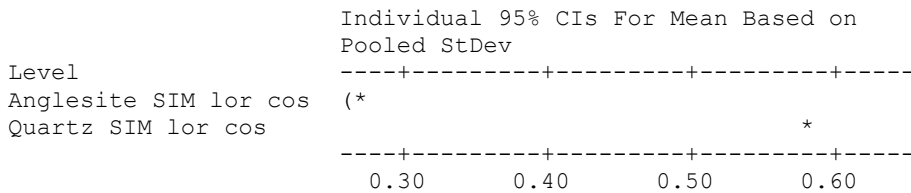
Pooled StDev = 0.01020

### One-way ANOVA: Anglesite SIM lor cos, Quartz SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.3168187	0.3168187	17399.36	0.000
Error	11	0.0002003	0.0000182		
Total	12	0.3170190			

S = 0.004267    R-Sq = 99.94%    R-Sq(adj) = 99.93%

Level	N	Mean	StDev
Anglesite SIM lor cos	6	0.26775	0.00518
Quartz SIM lor cos	7	0.58090	0.00332



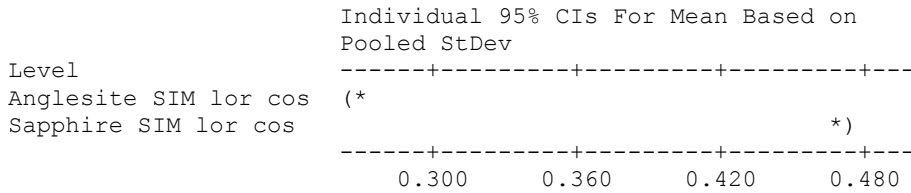
Pooled StDev = 0.00427

### One-way ANOVA: Anglesite SIM lor cos, Sapphire SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.1397609	0.1397609	5375.85	0.000
Error	12	0.0003120	0.0000260		
Total	13	0.1400729			

S = 0.005099    R-Sq = 99.78%    R-Sq(adj) = 99.76%

Level	N	Mean	StDev
Anglesite SIM lor cos	6	0.26775	0.00518
Sapphire SIM lor cos	8	0.46965	0.00504



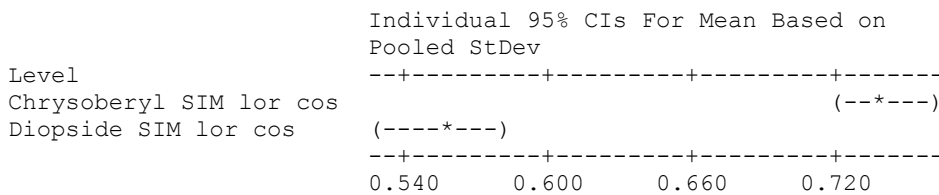
Pooled StDev = 0.00510

### One-way ANOVA: Chrysoberyl SIM lor cos, Diopside SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.19902	0.19902	117.72	0.000
Error	22	0.03720	0.00169		
Total	23	0.23622			

S = 0.04112    R-Sq = 84.25%    R-Sq(adj) = 83.54%

Level	N	Mean	StDev
Chrysoberyl SIM lor cos	14	0.74092	0.02275
Diopside SIM lor cos	10	0.55621	0.05819



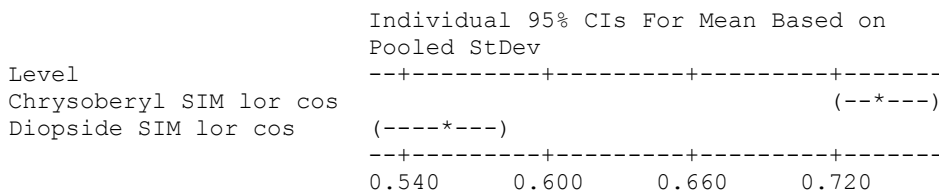
Pooled StDev = 0.04112

### One-way ANOVA: Chrysoberyl SIM lor cos, Diopside SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.19902	0.19902	117.72	0.000
Error	22	0.03720	0.00169		
Total	23	0.23622			

S = 0.04112    R-Sq = 84.25%    R-Sq(adj) = 83.54%

Level	N	Mean	StDev
Chrysoberyl SIM lor cos	14	0.74092	0.02275
Diopside SIM lor cos	10	0.55621	0.05819



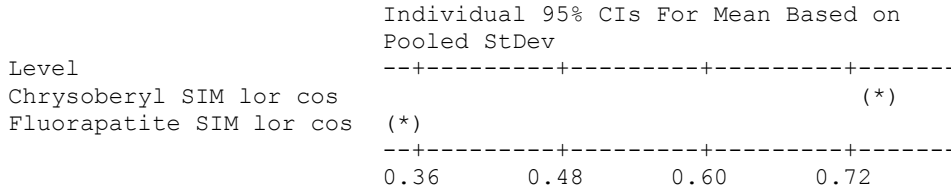
Pooled StDev = 0.04112

### One-way ANOVA: Chrysoberyl SIM lor cos, Fluorapatite SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.649197	0.649197	1648.38	0.000
Error	18	0.007089	0.000394		
Total	19	0.656286			

S = 0.01985 R-Sq = 98.92% R-Sq(adj) = 98.86%

Level	N	Mean	StDev
Chrysoberyl SIM lor cos	14	0.74092	0.02275
Fluorapatite SIM lor cos	6	0.34777	0.00853



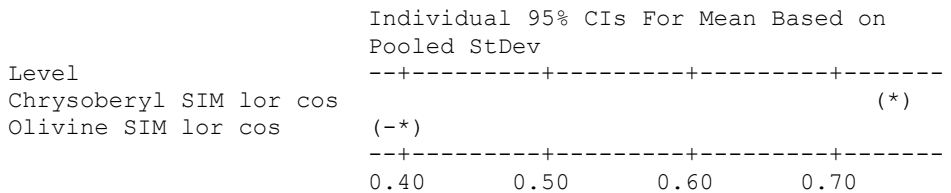
Pooled StDev = 0.01985

### One-way ANOVA: Chrysoberyl SIM lor cos, Olivine SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.499050	0.499050	1177.17	0.000
Error	18	0.007631	0.000424		
Total	19	0.506681			

S = 0.02059 R-Sq = 98.49% R-Sq(adj) = 98.41%

Level	N	Mean	StDev
Chrysoberyl SIM lor cos	14	0.74092	0.02275
Olivine SIM lor cos	6	0.39622	0.01346



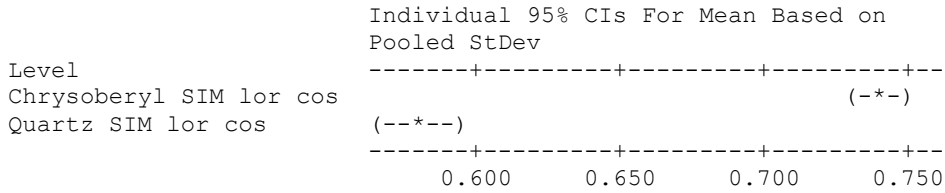
Pooled StDev = 0.02059

### One-way ANOVA: Chrysoberyl SIM lor cos, Quartz SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.119499	0.119499	334.31	0.000
Error	19	0.006792	0.000357		
Total	20	0.126290			

S = 0.01891 R-Sq = 94.62% R-Sq(adj) = 94.34%

Level	N	Mean	StDev
Chrysoberyl SIM lor cos	14	0.74092	0.02275
Quartz SIM lor cos	7	0.58090	0.00332



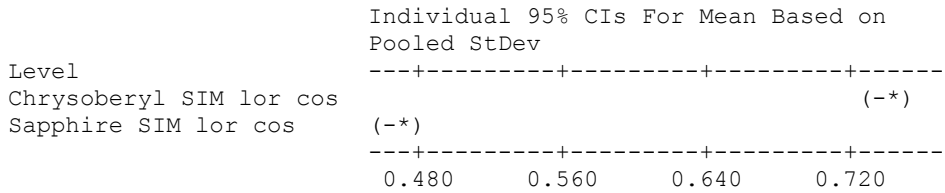
Pooled StDev = 0.01891

### One-way ANOVA: Chrysoberyl SIM lor cos, Sapphire SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.374631	0.374631	1085.38	0.000
Error	20	0.006903	0.000345		
Total	21	0.381534			

S = 0.01858 R-Sq = 98.19% R-Sq(adj) = 98.10%

Level	N	Mean	StDev
Chrysoberyl SIM lor cos	14	0.74092	0.02275
Sapphire SIM lor cos	8	0.46965	0.00504



Pooled StDev = 0.01858

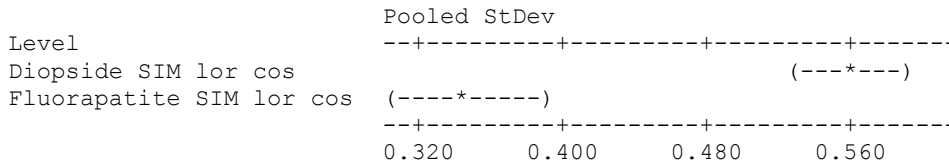
### One-way ANOVA: Diopside SIM lor cos, Fluorapatite SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.16293	0.16293	73.98	0.000
Error	14	0.03083	0.00220		
Total	15	0.19377			

S = 0.04693 R-Sq = 84.09% R-Sq(adj) = 82.95%

Level	N	Mean	StDev
Diopside SIM lor cos	10	0.55621	0.05819
Fluorapatite SIM lor cos	6	0.34777	0.00853

Individual 95% CIs For Mean Based on



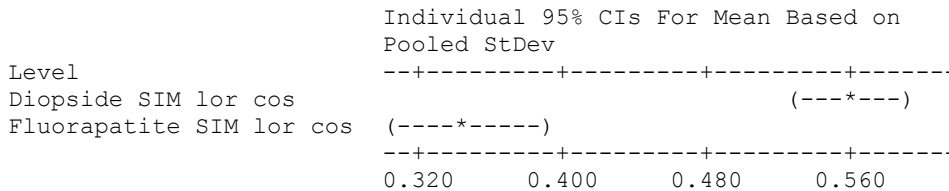
Pooled StDev = 0.04693

### One-way ANOVA: Diopside SIM lor cos, Fluorapatite SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.16293	0.16293	73.98	0.000
Error	14	0.03083	0.00220		
Total	15	0.19377			

S = 0.04693 R-Sq = 84.09% R-Sq(adj) = 82.95%

Level	N	Mean	StDev
Diopside SIM lor cos	10	0.55621	0.05819
Fluorapatite SIM lor cos	6	0.34777	0.00853



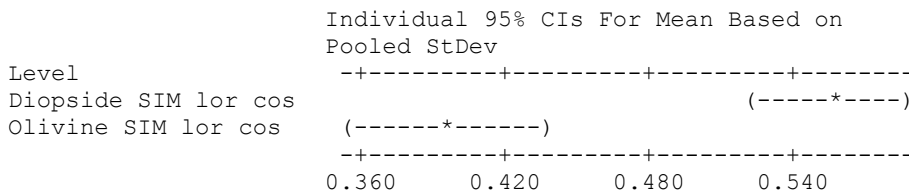
Pooled StDev = 0.04693

### One-way ANOVA: Diopside SIM lor cos, Olivine SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.09599	0.09599	42.83	0.000
Error	14	0.03138	0.00224		
Total	15	0.12737			

S = 0.04734 R-Sq = 75.37% R-Sq(adj) = 73.61%

Level	N	Mean	StDev
Diopside SIM lor cos	10	0.55621	0.05819
Olivine SIM lor cos	6	0.39622	0.01346



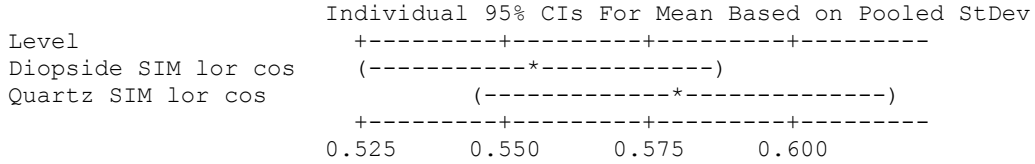
Pooled StDev = 0.04734

### One-way ANOVA: Diopside SIM lor cos, Quartz SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.00251	0.00251	1.23	0.284
Error	15	0.03054	0.00204		
Total	16	0.03305			

S = 0.04512    R-Sq = 7.60%    R-Sq(adj) = 1.44%

Level	N	Mean	StDev
Diopside SIM lor cos	10	0.55621	0.05819
Quartz SIM lor cos	7	0.58090	0.00332



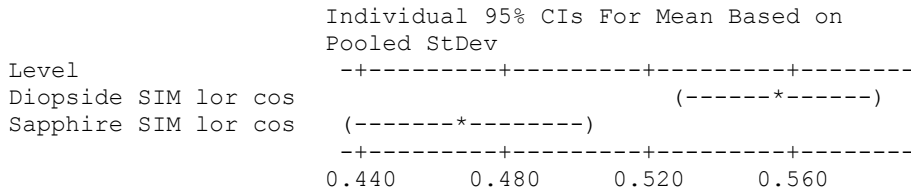
Pooled StDev = 0.04512

### One-way ANOVA: Diopside SIM lor cos, Sapphire SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.03330	0.03330	17.38	0.001
Error	16	0.03065	0.00192		
Total	17	0.06395			

S = 0.04377    R-Sq = 52.07%    R-Sq(adj) = 49.08%

Level	N	Mean	StDev
Diopside SIM lor cos	10	0.55621	0.05819
Sapphire SIM lor cos	8	0.46965	0.00504



Pooled StDev = 0.04377

### One-way ANOVA: Fluorapatite SIM lor cos, Olivine SIM lor cos

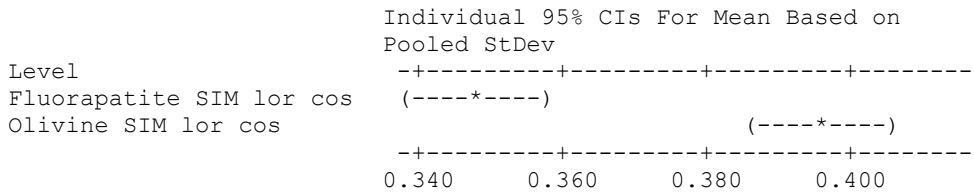
Source	DF	SS	MS	F	P
Factor	1	0.007042	0.007042	55.49	0.000
Error	10	0.001269	0.000127		
Total	11	0.008311			

S = 0.01126    R-Sq = 84.73%    R-Sq(adj) = 83.20%

Level	N	Mean	StDev
Fluorapatite SIM lor cos	6	0.34777	0.00853



Olivine SIM lor cos 6 0.39622 0.01346



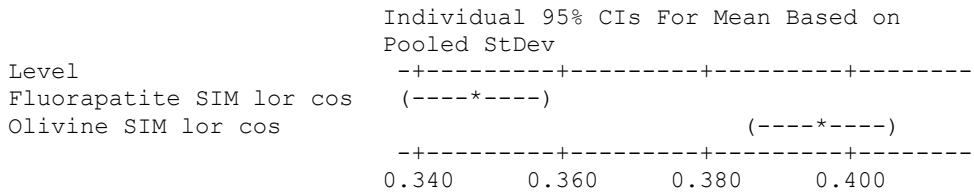
Pooled StDev = 0.01126

**One-way ANOVA: Fluorapatite SIM lor cos, Olivine SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.007042	0.007042	55.49	0.000
Error	10	0.001269	0.000127		
Total	11	0.008311			

S = 0.01126 R-Sq = 84.73% R-Sq(adj) = 83.20%

Level	N	Mean	StDev
Fluorapatite SIM lor cos	6	0.34777	0.00853
Olivine SIM lor cos	6	0.39622	0.01346



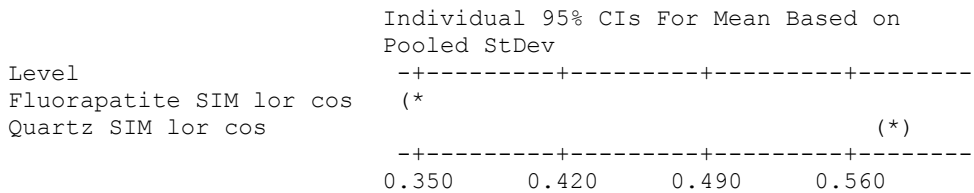
Pooled StDev = 0.01126

**One-way ANOVA: Fluorapatite SIM lor cos, Quartz SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.1755960	0.1755960	4495.83	0.000
Error	11	0.0004296	0.0000391		
Total	12	0.1760257			

S = 0.006250 R-Sq = 99.76% R-Sq(adj) = 99.73%

Level	N	Mean	StDev
Fluorapatite SIM lor cos	6	0.34777	0.00853
Quartz SIM lor cos	7	0.58090	0.00332



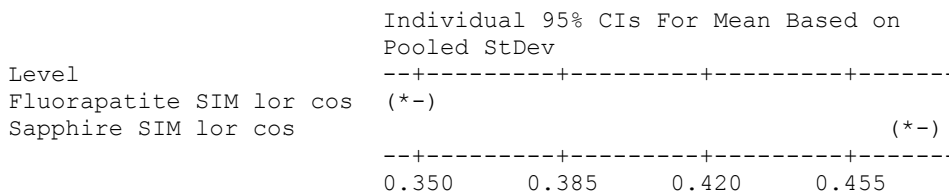
Pooled StDev = 0.00625

**One-way ANOVA: Fluorapatite SIM lor cos, Sapphire SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.0509333	0.0509333	1129.11	0.000
Error	12	0.0005413	0.0000451		
Total	13	0.0514746			

S = 0.006716    R-Sq = 98.95%    R-Sq(adj) = 98.86%

Level	N	Mean	StDev
Fluorapatite SIM lor cos	6	0.34777	0.00853
Sapphire SIM lor cos	8	0.46965	0.00504



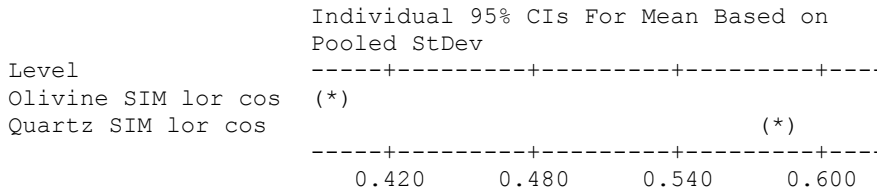
Pooled StDev = 0.00672

**One-way ANOVA: Olivine SIM lor cos, Quartz SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.1101949	0.1101949	1247.77	0.000
Error	11	0.0009714	0.0000883		
Total	12	0.1111663			

S = 0.009398    R-Sq = 99.13%    R-Sq(adj) = 99.05%

Level	N	Mean	StDev
Olivine SIM lor cos	6	0.39622	0.01346
Quartz SIM lor cos	7	0.58090	0.00332



Pooled StDev = 0.00940

**One-way ANOVA: Olivine SIM lor cos, Sapphire SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.0184884	0.0184884	204.83	0.000
Error	12	0.0010831	0.0000903		
Total	13	0.0195715			

S = 0.009501    R-Sq = 94.47%    R-Sq(adj) = 94.00%

Level	N	Mean	StDev
Olivine SIM lor cos	6	0.39622	0.01346
Sapphire SIM lor cos	8	0.46965	0.00504

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Olivine SIM lor cos	(--*--)
Sapphire SIM lor cos	(--*--)

0.400      0.425      0.450      0.475

Pooled StDev = 0.00950

### One-way ANOVA: Quartz SIM lor cos, Sapphire SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.0462058	0.0462058	2464.21	0.000
Error	13	0.0002438	0.0000188		
Total	14	0.0464496			

S = 0.004330    R-Sq = 99.48%    R-Sq(adj) = 99.43%

Level	N	Mean	StDev
Quartz SIM lor cos	7	0.58090	0.00332
Sapphire SIM lor cos	8	0.46965	0.00504

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Quartz SIM lor cos	(-*)
Sapphire SIM lor cos	(-*)

0.480      0.510      0.540      0.570

Pooled StDev = 0.00433

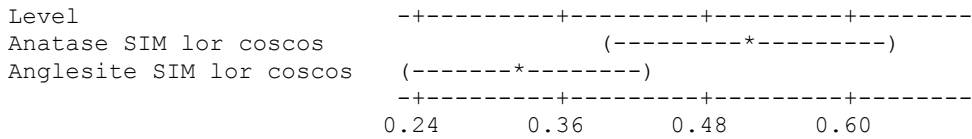
### One-way ANOVA: Anatase SIM lor coscos, Anglesite SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.0859	0.0859	7.39	0.026
Error	8	0.0930	0.0116		
Total	9	0.1789			

S = 0.1078    R-Sq = 48.02%    R-Sq(adj) = 41.52%

Level	N	Mean	StDev
Anatase SIM lor coscos	4	0.5177	0.1761
Anglesite SIM lor coscos	6	0.3285	0.0020

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.1078

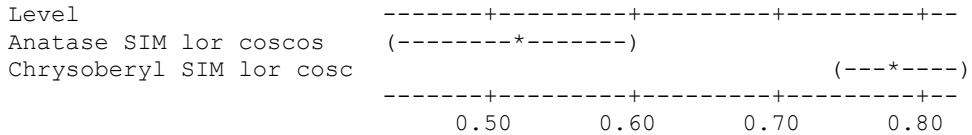
**One-way ANOVA: Anatase SIM lor coscos, Chrysoberyl SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.22004	0.22004	33.30	0.000
Error	16	0.10574	0.00661		
Total	17	0.32578			

S = 0.08129    R-Sq = 67.54%    R-Sq(adj) = 65.51%

Level	N	Mean	StDev
Anatase SIM lor coscos	4	0.51768	0.17606
Chrysoberyl SIM lor cosc	14	0.78362	0.03132

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.08129

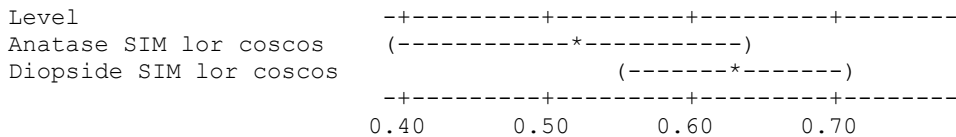
**One-way ANOVA: Anatase SIM lor coscos, Diopside SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.0371	0.0371	2.75	0.123
Error	12	0.1621	0.0135		
Total	13	0.1992			

S = 0.1162    R-Sq = 18.64%    R-Sq(adj) = 11.87%

Level	N	Mean	StDev
Anatase SIM lor coscos	4	0.5177	0.1761
Diopside SIM lor coscos	10	0.6317	0.0876

Individual 95% CIs For Mean Based on Pooled StDev



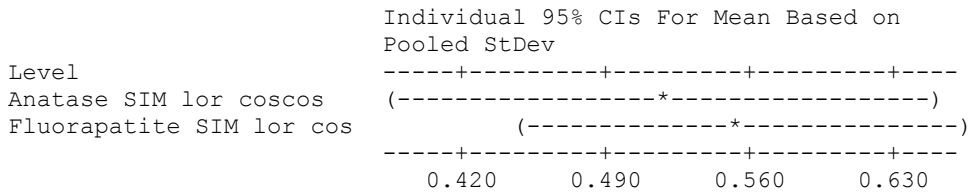
Pooled StDev = 0.1162

**One-way ANOVA: Anatase SIM lor coscos, Fluorapatite SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.0033	0.0033	0.25	0.633
Error	8	0.1057	0.0132		
Total	9	0.1090			

S = 0.1149    R-Sq = 2.99%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Anatase SIM lor coscos	4	0.5177	0.1761
Fluorapatite SIM lor cos	6	0.5545	0.0504



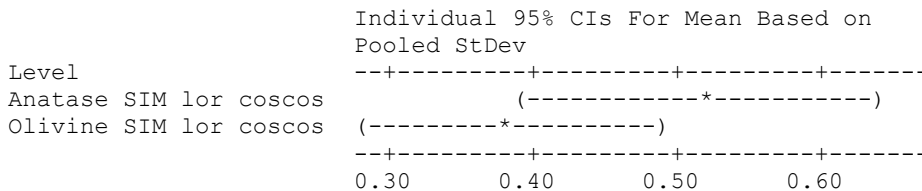
Pooled StDev = 0.1149

**One-way ANOVA: Anatase SIM lor coscos, Olivine SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.0433	0.0433	3.61	0.094
Error	8	0.0958	0.0120		
Total	9	0.1390			

S = 0.1094    R-Sq = 31.11%    R-Sq(adj) = 22.50%

Level	N	Mean	StDev
Anatase SIM lor coscos	4	0.5177	0.1761
Olivine SIM lor coscos	6	0.3834	0.0236



Pooled StDev = 0.1094

**One-way ANOVA: Anatase SIM lor coscos, Quartz SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.1000	0.1000	9.67	0.013
Error	9	0.0931	0.0103		
Total	10	0.1930			

S = 0.1017    R-Sq = 51.79%    R-Sq(adj) = 46.43%

Level	N	Mean	StDev
Anatase SIM lor coscos	4	0.5177	0.1761
Quartz SIM lor coscos	7	0.7159	0.0037

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Anatase SIM lor coscos	(-----*-----)	
Quartz SIM lor coscos		(-----*-----)

0.48      0.60      0.72      0.84

Pooled StDev = 0.1017

### One-way ANOVA: Anatase SIM lor coscos, Sapphire SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.00446	0.00446	0.48	0.505
Error	10	0.09325	0.00933		
Total	11	0.09771			

S = 0.09657    R-Sq = 4.56%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Anatase SIM lor coscos	4	0.51768	0.17606
Sapphire SIM lor coscos	8	0.55855	0.00615

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Anatase SIM lor coscos	(-----*-----)	
Sapphire SIM lor coscos		(-----*-----)

0.420      0.480      0.540      0.600

Pooled StDev = 0.09657

### One-way ANOVA: Anglesite SIM lor coscos, Chrysoberyl SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.870097	0.870097	1226.59	0.000
Error	18	0.012768	0.000709		
Total	19	0.882865			

S = 0.02663    R-Sq = 98.55%    R-Sq(adj) = 98.47%

Level	N	Mean	StDev
Anglesite SIM lor coscos	6	0.32847	0.00195
Chrysoberyl SIM lor cosc	14	0.78362	0.03132

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Anglesite SIM lor coscos	(-*)	
Chrysoberyl SIM lor cosc		(*)

0.30      0.45      0.60      0.75

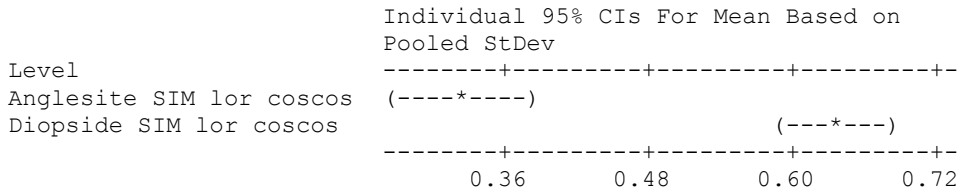
Pooled StDev = 0.02663

### One-way ANOVA: Anglesite SIM lor coscos, Diopside SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.34481	0.34481	69.84	0.000
Error	14	0.06913	0.00494		
Total	15	0.41394			

S = 0.07027 R-Sq = 83.30% R-Sq(adj) = 82.11%

Level	N	Mean	StDev
Anglesite SIM lor coscos	6	0.32847	0.00195
Diopside SIM lor coscos	10	0.63170	0.08763



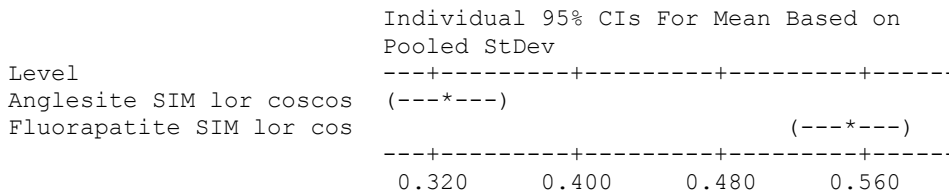
Pooled StDev = 0.07027

### One-way ANOVA: Anglesite SIM lor coscos, Fluorapatite SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.15330	0.15330	120.39	0.000
Error	10	0.01273	0.00127		
Total	11	0.16603			

S = 0.03568 R-Sq = 92.33% R-Sq(adj) = 91.56%

Level	N	Mean	StDev
Anglesite SIM lor coscos	6	0.32847	0.00195
Fluorapatite SIM lor cos	6	0.55452	0.05043



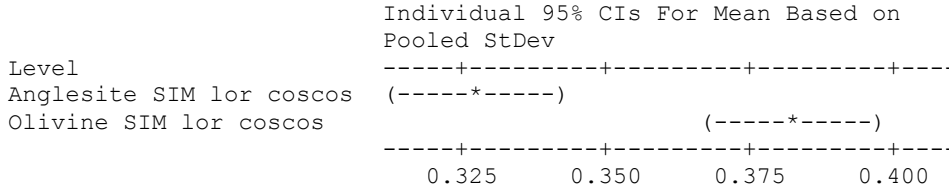
Pooled StDev = 0.03568

### One-way ANOVA: Anglesite SIM lor coscos, Olivine SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.009059	0.009059	32.25	0.000
Error	10	0.002809	0.000281		
Total	11	0.011868			

S = 0.01676 R-Sq = 76.33% R-Sq(adj) = 73.96%

Level	N	Mean	StDev
Anglesite SIM lor coscos	6	0.32847	0.00195
Olivine SIM lor coscos	6	0.38342	0.02362



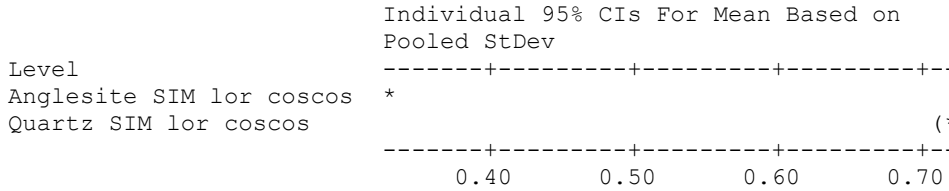
Pooled StDev = 0.01676

### One-way ANOVA: Anglesite SIM lor coscos, Quartz SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.4848460	0.4848460	53115.04	0.000
Error	11	0.0001004	0.0000091		
Total	12	0.4849464			

S = 0.003021 R-Sq = 99.98% R-Sq(adj) = 99.98%

Level	N	Mean	StDev
Anglesite SIM lor coscos	6	0.32847	0.00195
Quartz SIM lor coscos	7	0.71586	0.00368



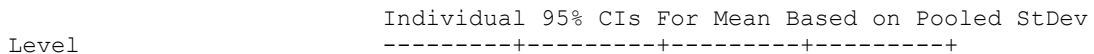
Pooled StDev = 0.00302

### One-way ANOVA: Anglesite SIM lor coscos, Sapphire SIM lor cos

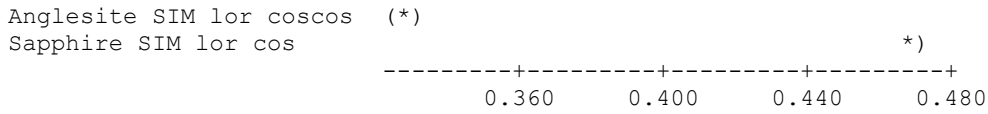
Source	DF	SS	MS	F	P
Factor	1	0.0683408	0.0683408	4168.11	0.000
Error	12	0.0001968	0.0000164		
Total	13	0.0685376			

S = 0.004049 R-Sq = 99.71% R-Sq(adj) = 99.69%

Level	N	Mean	StDev
Anglesite SIM lor coscos	6	0.32847	0.00195
Sapphire SIM lor cos	8	0.46965	0.00504







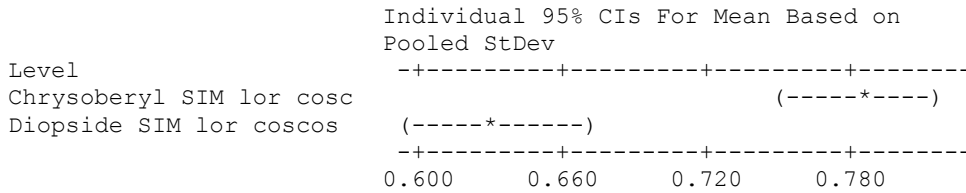
Pooled StDev = 0.00405

**One-way ANOVA: Chrysoberyl SIM lor coscos, Diopside SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.13463	0.13463	36.19	0.000
Error	22	0.08186	0.00372		
Total	23	0.21649			

S = 0.06100 R-Sq = 62.19% R-Sq(adj) = 60.47%

Level	N	Mean	StDev
Chrysoberyl SIM lor cosc	14	0.78362	0.03132
Diopside SIM lor coscos	10	0.63170	0.08763



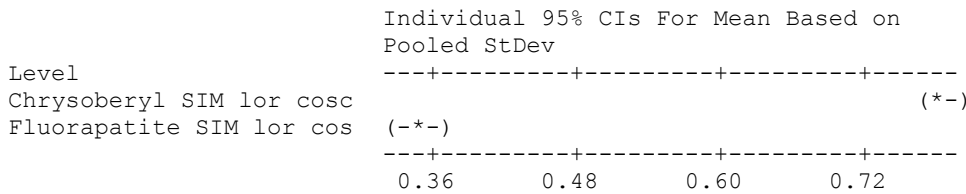
Pooled StDev = 0.06100

**One-way ANOVA: Chrysoberyl SIM lor coscos, Fluorapatite SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.797871	0.797871	1095.22	0.000
Error	18	0.013113	0.000729		
Total	19	0.810984			

S = 0.02699 R-Sq = 98.38% R-Sq(adj) = 98.29%

Level	N	Mean	StDev
Chrysoberyl SIM lor cosc	14	0.78362	0.03132
Fluorapatite SIM lor cos	6	0.34777	0.00853



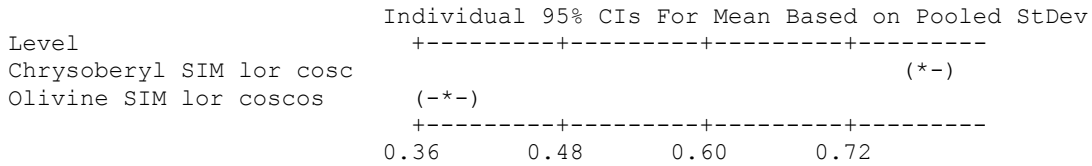
Pooled StDev = 0.02699

### One-way ANOVA: Chrysoberyl SIM lor coscos, Olivine SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.672688	0.672688	779.20	0.000
Error	18	0.015539	0.000863		
Total	19	0.688228			

S = 0.02938 R-Sq = 97.74% R-Sq(adj) = 97.62%

Level	N	Mean	StDev
Chrysoberyl SIM lor cosc	14	0.78362	0.03132
Olivine SIM lor coscos	6	0.38342	0.02362



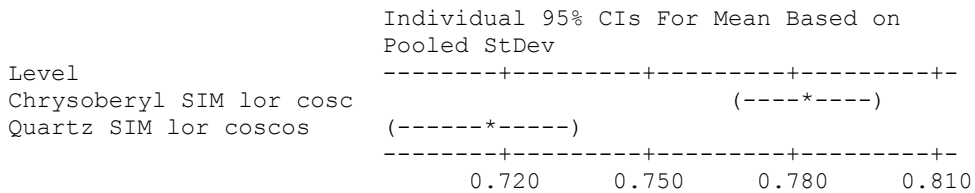
Pooled StDev = 0.02938

### One-way ANOVA: Chrysoberyl SIM lor coscos, Quartz SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.021429	0.021429	31.73	0.000
Error	19	0.012831	0.000675		
Total	20	0.034260			

S = 0.02599 R-Sq = 62.55% R-Sq(adj) = 60.58%

Level	N	Mean	StDev
Chrysoberyl SIM lor cosc	14	0.78362	0.03132
Quartz SIM lor coscos	7	0.71586	0.00368



Pooled StDev = 0.02599

### One-way ANOVA: Chrysoberyl SIM lor coscos, Sapphire SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.257891	0.257891	396.33	0.000
Error	20	0.013014	0.000651		
Total	21	0.270905			

S = 0.02551 R-Sq = 95.20% R-Sq(adj) = 94.96%

Level	N	Mean	StDev
Chrysoberyl SIM lor cosc	14	0.78362	0.03132
Sapphire SIM lor coscos	8	0.55855	0.00615

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Chrysoberyl SIM lor cosc	0.72	0.85
Sapphire SIM lor coscos	0.53	0.59

Pooled StDev = 0.02551

### One-way ANOVA: Diopside SIM lor coscos, Fluorapatite SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.02234	0.02234	3.82	0.071
Error	14	0.08182	0.00584		
Total	15	0.10416			

S = 0.07645 R-Sq = 21.45% R-Sq(adj) = 15.84%

Level	N	Mean	StDev
Diopside SIM lor coscos	10	0.63170	0.08763
Fluorapatite SIM lor cos	6	0.55452	0.05043

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Diopside SIM lor coscos	0.54	0.72
Fluorapatite SIM lor cos	0.50	0.61

Pooled StDev = 0.07645

### One-way ANOVA: Diopside SIM lor coscos, Olivine SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.23117	0.23117	45.01	0.000
Error	14	0.07190	0.00514		
Total	15	0.30306			

S = 0.07166 R-Sq = 76.28% R-Sq(adj) = 74.58%

Level	N	Mean	StDev
Diopside SIM lor coscos	10	0.63170	0.08763
Olivine SIM lor coscos	6	0.38342	0.02362

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Diopside SIM lor coscos	0.54	0.72
Olivine SIM lor coscos	0.36	0.41

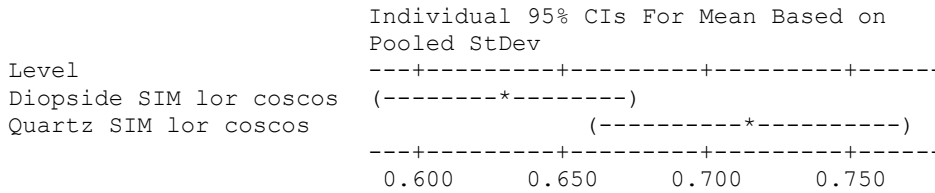
Pooled StDev = 0.07166

### One-way ANOVA: Diopside SIM lor coscos, Quartz SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.02916	0.02916	6.32	0.024
Error	15	0.06919	0.00461		
Total	16	0.09835			

S = 0.06792 R-Sq = 29.65% R-Sq(adj) = 24.96%

Level	N	Mean	StDev
Diopside SIM lor coscos	10	0.63170	0.08763
Quartz SIM lor coscos	7	0.71586	0.00368



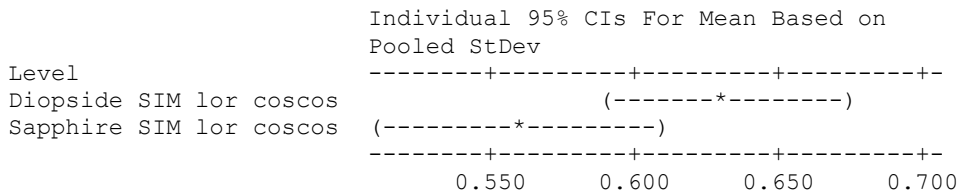
Pooled StDev = 0.06792

### One-way ANOVA: Diopside SIM lor coscos, Sapphire SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.02378	0.02378	5.49	0.032
Error	16	0.06937	0.00434		
Total	17	0.09315			

S = 0.06585 R-Sq = 25.53% R-Sq(adj) = 20.88%

Level	N	Mean	StDev
Diopside SIM lor coscos	10	0.63170	0.08763
Sapphire SIM lor coscos	8	0.55855	0.00615



Pooled StDev = 0.06585

### One-way ANOVA: Fluorapatite SIM lor coscos, Olivine SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.08783	0.08783	56.65	0.000
Error	10	0.01550	0.00155		
Total	11	0.10333			

S = 0.03938 R-Sq = 85.00% R-Sq(adj) = 83.49%

Level	N	Mean	StDev
Fluorapatite SIM lor cos	6	0.55452	0.05043
Olivine SIM lor coscos	6	0.38342	0.02362

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Fluorapatite SIM lor cos	0.420	0.689
Olivine SIM lor coscos	0.350	0.417

Pooled StDev = 0.03938

### One-way ANOVA: Fluorapatite SIM lor coscos, Quartz SIM coscos

Source	DF	SS	MS	F	P
Factor	1	0.0004	0.0004	0.03	0.857
Error	11	0.1434	0.0130		
Total	12	0.1439			

S = 0.1142 R-Sq = 0.31% R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Fluorapatite SIM lor cos	6	0.5545	0.0504
Quartz SIM coscos	7	0.5428	0.1476

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Fluorapatite SIM lor cos	0.480	0.630
Quartz SIM coscos	0.480	0.600

Pooled StDev = 0.1142

### One-way ANOVA: Fluorapatite SIM lor coscos, Sapphire SIM lor coscos

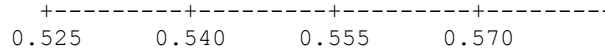
Source	DF	SS	MS	F	P
Factor	1	0.00006	0.00006	0.05	0.824
Error	12	0.01298	0.00108		
Total	13	0.01303			

S = 0.03289 R-Sq = 0.43% R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Fluorapatite SIM lor cos	6	0.55452	0.05043
Sapphire SIM lor coscos	8	0.55855	0.00615

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Fluorapatite SIM lor cos	0.480	0.630
Sapphire SIM lor coscos	0.550	0.567



Pooled StDev = 0.03289

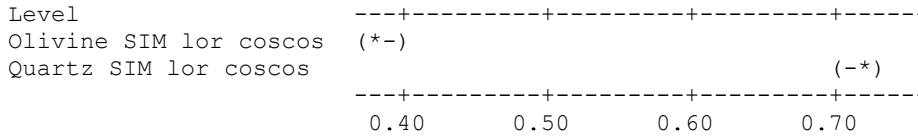
**One-way ANOVA: Olivine SIM lor coscos, Quartz SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.357054	0.357054	1367.85	0.000
Error	11	0.002871	0.000261		
Total	12	0.359925			

S = 0.01616    R-Sq = 99.20%    R-Sq(adj) = 99.13%

Level	N	Mean	StDev
Olivine SIM lor coscos	6	0.38342	0.02362
Quartz SIM lor coscos	7	0.71586	0.00368

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.01616

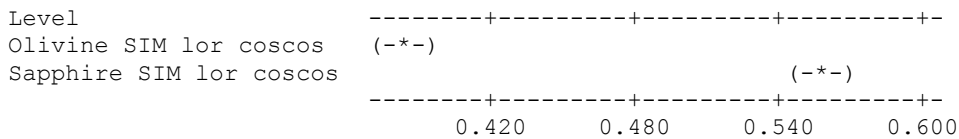
**One-way ANOVA: Olivine SIM lor coscos, Sapphire SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.105160	0.105160	413.16	0.000
Error	12	0.003054	0.000255		
Total	13	0.108214			

S = 0.01595    R-Sq = 97.18%    R-Sq(adj) = 96.94%

Level	N	Mean	StDev
Olivine SIM lor coscos	6	0.38342	0.02362
Sapphire SIM lor coscos	8	0.55855	0.00615

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.01595

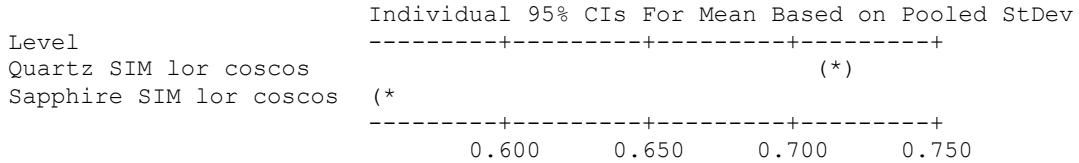
**One-way ANOVA: Quartz SIM lor coscos, Sapphire SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.0923833	0.0923833	3473.69	0.000

Error 13 0.0003457 0.0000266  
 Total 14 0.0927291

S = 0.005157 R-Sq = 99.63% R-Sq(adj) = 99.60%

Level	N	Mean	StDev
Quartz SIM lor coscos	7	0.71586	0.00368
Sapphire SIM lor coscos	8	0.55855	0.00615



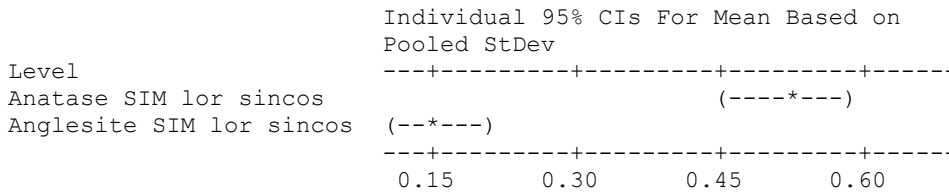
Pooled StDev = 0.00516

### One-way ANOVA: Anatase SIM lor sincos, Anglesite SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.32719	0.32719	106.08	0.000
Error	8	0.02467	0.00308		
Total	9	0.35186			

S = 0.05554 R-Sq = 92.99% R-Sq(adj) = 92.11%

Level	N	Mean	StDev
Anatase SIM lor sincos	4	0.51992	0.08552
Anglesite SIM lor sincos	6	0.15070	0.02338



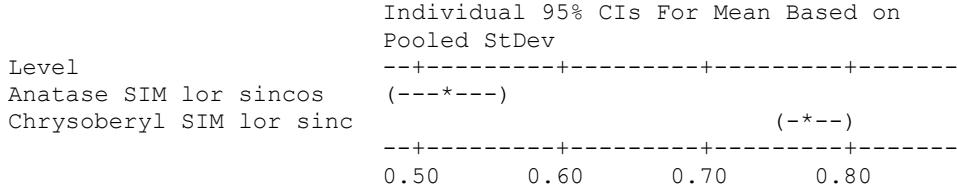
Pooled StDev = 0.05554

### One-way ANOVA: Anatase SIM lor sincos, Chrysoberyl SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.19849	0.19849	114.90	0.000
Error	16	0.02764	0.00173		
Total	17	0.22613			

S = 0.04156 R-Sq = 87.78% R-Sq(adj) = 87.01%

Level	N	Mean	StDev
Anatase SIM lor sincos	4	0.51992	0.08552
Chrysoberyl SIM lor sinc	14	0.77251	0.02094



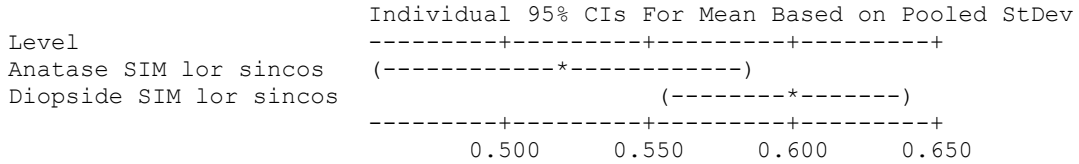
Pooled StDev = 0.04156

**One-way ANOVA: Anatase SIM lor sincos, Diopside SIM lor sincos**

Source	DF	SS	MS	F	P
Factor	1	0.01733	0.01733	4.56	0.054
Error	12	0.04556	0.00380		
Total	13	0.06289			

S = 0.06162 R-Sq = 27.55% R-Sq(adj) = 21.52%

Level	N	Mean	StDev
Anatase SIM lor sincos	4	0.51992	0.08552
Diopside SIM lor sincos	10	0.59780	0.05123



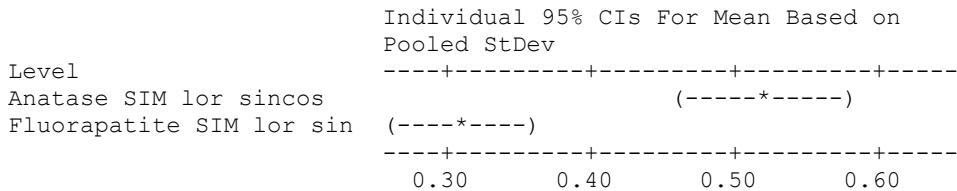
Pooled StDev = 0.06162

**One-way ANOVA: Anatase SIM lor sincos, Fluorapatite SIM lor sincos**

Source	DF	SS	MS	F	P
Factor	1	0.11007	0.11007	38.25	0.000
Error	8	0.02302	0.00288		
Total	9	0.13310			

S = 0.05364 R-Sq = 82.70% R-Sq(adj) = 80.54%

Level	N	Mean	StDev
Anatase SIM lor sincos	4	0.51992	0.08552
Fluorapatite SIM lor sin	6	0.30577	0.01470



Pooled StDev = 0.05364

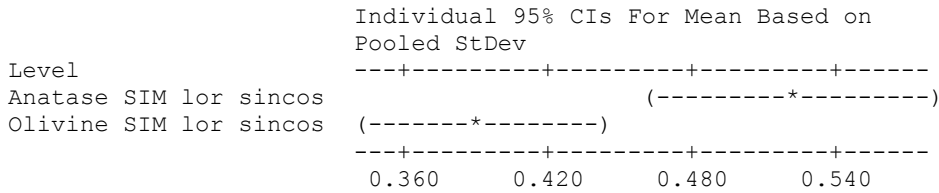
**One-way ANOVA: Anatase SIM lor sincos, Olivine SIM lor sincos**



Source	DF	SS	MS	F	P
Factor	1	0.03900	0.03900	14.09	0.006
Error	8	0.02214	0.00277		
Total	9	0.06114			

S = 0.05261 R-Sq = 63.79% R-Sq(adj) = 59.26%

Level	N	Mean	StDev
Anatase SIM lor sincos	4	0.51992	0.08552
Olivine SIM lor sincos	6	0.39245	0.00632



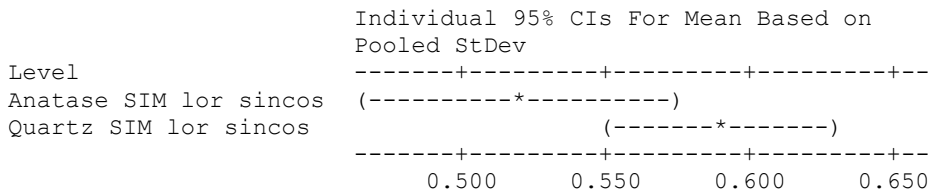
Pooled StDev = 0.05261

### One-way ANOVA: Anatase SIM lor sincos, Quartz SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.01248	0.01248	5.10	0.050
Error	9	0.02202	0.00245		
Total	10	0.03450			

S = 0.04946 R-Sq = 36.18% R-Sq(adj) = 29.08%

Level	N	Mean	StDev
Anatase SIM lor sincos	4	0.51992	0.08552
Quartz SIM lor sincos	7	0.58994	0.00354



Pooled StDev = 0.04946

### One-way ANOVA: Anatase SIM lor sincos, Sapphire SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.00518	0.00518	2.31	0.160
Error	10	0.02244	0.00224		
Total	11	0.02762			

S = 0.04737 R-Sq = 18.75% R-Sq(adj) = 10.63%

Level	N	Mean	StDev
Anatase SIM lor sincos	4	0.51992	0.08552
Sapphire SIM lor sincos	8	0.47585	0.00847

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anatase SIM lor sincos	(-----*-----)
Sapphire SIM lor sincos	(-----*-----)

0.455      0.490      0.525      0.560

Pooled StDev = 0.04737

### One-way ANOVA: Anglesite SIM lor sincos, Chrysoberyl SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	1.623943	1.623943	3466.45	0.000
Error	18	0.008433	0.000468		
Total	19	1.632375			

S = 0.02164    R-Sq = 99.48%    R-Sq(adj) = 99.45%

Level	N	Mean	StDev
Anglesite SIM lor sincos	6	0.15070	0.02338
Chrysoberyl SIM lor sinc	14	0.77251	0.02094

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anglesite SIM lor sincos	(*
Chrysoberyl SIM lor sinc	(*)

0.20      0.40      0.60      0.80

Pooled StDev = 0.02164

### One-way ANOVA: Anglesite SIM lor sincos, Diopside SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.74962	0.74962	398.28	0.000
Error	14	0.02635	0.00188		
Total	15	0.77597			

S = 0.04338    R-Sq = 96.60%    R-Sq(adj) = 96.36%

Level	N	Mean	StDev
Anglesite SIM lor sincos	6	0.15070	0.02338
Diopside SIM lor sincos	10	0.59780	0.05123

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anglesite SIM lor sincos	(-*--)
Diopside SIM lor sincos	(-*--)

0.15      0.30      0.45      0.60

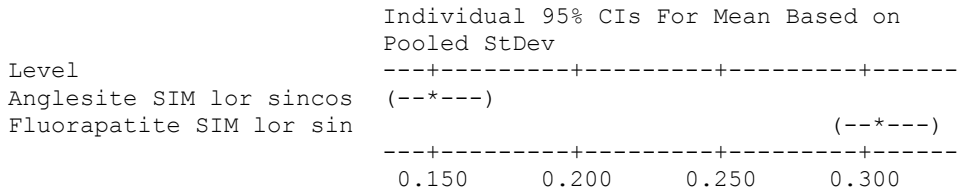
Pooled StDev = 0.04338

### One-way ANOVA: Anglesite SIM lor sincos, Fluorapatite SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.072137	0.072137	189.18	0.000
Error	10	0.003813	0.000381		
Total	11	0.075950			

S = 0.01953 R-Sq = 94.98% R-Sq(adj) = 94.48%

Level	N	Mean	StDev
Anglesite SIM lor sincos	6	0.15070	0.02338
Fluorapatite SIM lor sin	6	0.30577	0.01470



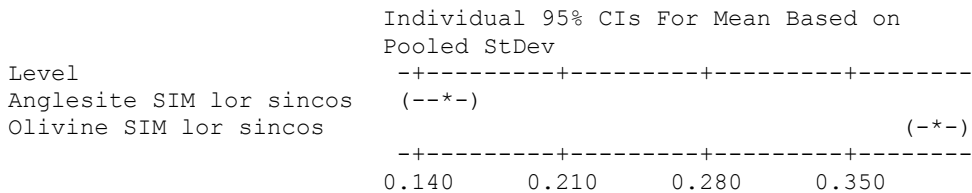
Pooled StDev = 0.01953

### One-way ANOVA: Anglesite SIM lor sincos, Olivine SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.175329	0.175329	598.01	0.000
Error	10	0.002932	0.000293		
Total	11	0.178261			

S = 0.01712 R-Sq = 98.36% R-Sq(adj) = 98.19%

Level	N	Mean	StDev
Anglesite SIM lor sincos	6	0.15070	0.02338
Olivine SIM lor sincos	6	0.39245	0.00632



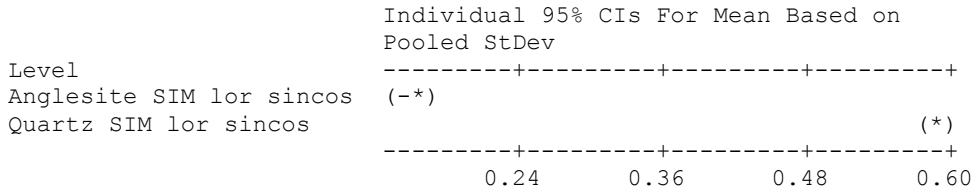
Pooled StDev = 0.01712

### One-way ANOVA: Anglesite SIM lor sincos, Quartz SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.623326	0.623326	2442.40	0.000
Error	11	0.002807	0.000255		
Total	12	0.626133			

S = 0.01598 R-Sq = 99.55% R-Sq(adj) = 99.51%

Level	N	Mean	StDev
Anglesite SIM lor sincos	6	0.15070	0.02338
Quartz SIM lor sincos	7	0.58994	0.00354



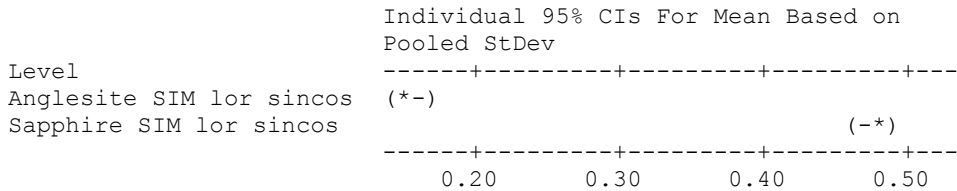
Pooled StDev = 0.01598

### One-way ANOVA: Anglesite SIM lor sincos, Sapphire SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.362477	0.362477	1344.61	0.000
Error	12	0.003235	0.000270		
Total	13	0.365712			

S = 0.01642 R-Sq = 99.12% R-Sq(adj) = 99.04%

Level	N	Mean	StDev
Anglesite SIM lor sincos	6	0.15070	0.02338
Sapphire SIM lor sincos	8	0.47585	0.00847



Pooled StDev = 0.01642

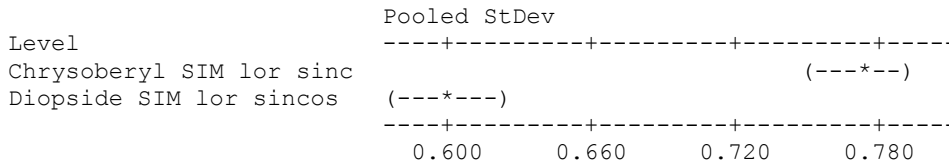
### One-way ANOVA: Chrysoberyl SIM lor sincos, Diopside SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.17806	0.17806	133.62	0.000
Error	22	0.02932	0.00133		
Total	23	0.20738			

S = 0.03651 R-Sq = 85.86% R-Sq(adj) = 85.22%

Level	N	Mean	StDev
Chrysoberyl SIM lor sinc	14	0.77251	0.02094
Diopside SIM lor sincos	10	0.59780	0.05123

Individual 95% CIs For Mean Based on



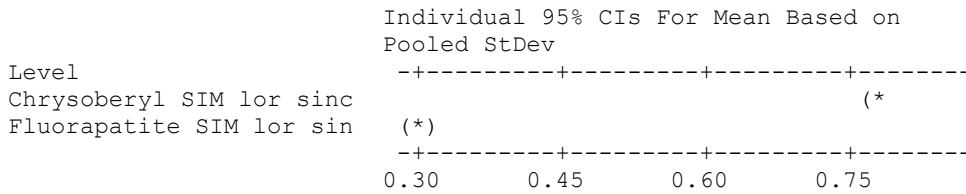
Pooled StDev = 0.03651

### One-way ANOVA: Chrysoberyl SIM lor sincos, Fluorapatite SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.914984	0.914984	2428.78	0.000
Error	18	0.006781	0.000377		
Total	19	0.921765			

S = 0.01941 R-Sq = 99.26% R-Sq(adj) = 99.22%

Level	N	Mean	StDev
Chrysoberyl SIM lor sinc	14	0.77251	0.02094
Fluorapatite SIM lor sin	6	0.30577	0.01470



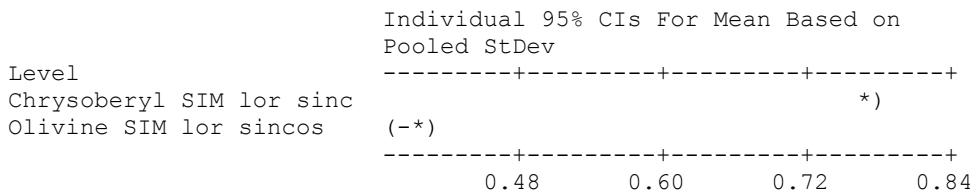
Pooled StDev = 0.01941

### One-way ANOVA: Chrysoberyl SIM lor sincos, Olivine SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.606685	0.606685	1850.97	0.000
Error	18	0.005900	0.000328		
Total	19	0.612585			

S = 0.01810 R-Sq = 99.04% R-Sq(adj) = 98.98%

Level	N	Mean	StDev
Chrysoberyl SIM lor sinc	14	0.77251	0.02094
Olivine SIM lor sincos	6	0.39245	0.00632



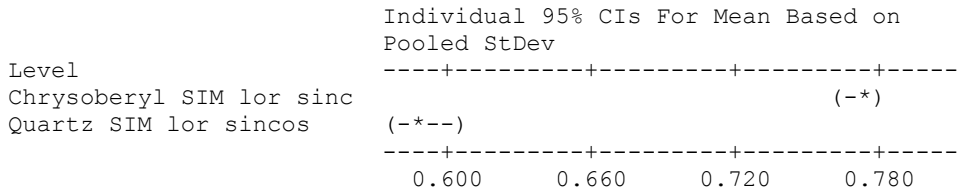
Pooled StDev = 0.01810

### One-way ANOVA: Chrysoberyl SIM lor sincos, Quartz SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.155551	0.155551	511.75	0.000
Error	19	0.005775	0.000304		
Total	20	0.161326			

S = 0.01743    R-Sq = 96.42%    R-Sq(adj) = 96.23%

Level	N	Mean	StDev
Chrysoberyl SIM lor sinc	14	0.77251	0.02094
Quartz SIM lor sincos	7	0.58994	0.00354



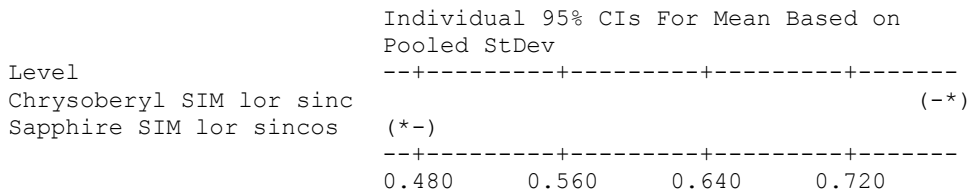
Pooled StDev = 0.01743

### One-way ANOVA: Chrysoberyl SIM lor sincos, Sapphire SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.448049	0.448049	1444.65	0.000
Error	20	0.006203	0.000310		
Total	21	0.454252			

S = 0.01761    R-Sq = 98.63%    R-Sq(adj) = 98.57%

Level	N	Mean	StDev
Chrysoberyl SIM lor sinc	14	0.77251	0.02094
Sapphire SIM lor sincos	8	0.47585	0.00847



Pooled StDev = 0.01761

### One-way ANOVA: Diopside SIM lor sincos, Fluorapatite SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.31981	0.31981	181.28	0.000
Error	14	0.02470	0.00176		
Total	15	0.34451			

S = 0.04200    R-Sq = 92.83%    R-Sq(adj) = 92.32%

Level	N	Mean	StDev
Diopside SIM lor sincos	10	0.59780	0.05123
Fluorapatite SIM lor sin	6	0.30577	0.01470

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Diopside SIM lor sincos	(--*--)
Fluorapatite SIM lor sin	(---*--)

0.30      0.40      0.50      0.60

Pooled StDev = 0.04200

### One-way ANOVA: Diopside SIM lor sincos, Fluorapatite SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.31981	0.31981	181.28	0.000
Error	14	0.02470	0.00176		
Total	15	0.34451			

S = 0.04200    R-Sq = 92.83%    R-Sq(adj) = 92.32%

Level	N	Mean	StDev
Diopside SIM lor sincos	10	0.59780	0.05123
Fluorapatite SIM lor sin	6	0.30577	0.01470

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Diopside SIM lor sincos	(--*--)
Fluorapatite SIM lor sin	(---*--)

0.30      0.40      0.50      0.60

Pooled StDev = 0.04200

### One-way ANOVA: Diopside SIM lor sincos, Olivine SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.15813	0.15813	92.95	0.000
Error	14	0.02382	0.00170		
Total	15	0.18195			

S = 0.04125    R-Sq = 86.91%    R-Sq(adj) = 85.97%

Level	N	Mean	StDev
Diopside SIM lor sincos	10	0.59780	0.05123
Olivine SIM lor sincos	6	0.39245	0.00632

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Diopside SIM lor sincos	(---*---)
Olivine SIM lor sincos	(----*----)

0.420      0.490      0.560      0.630

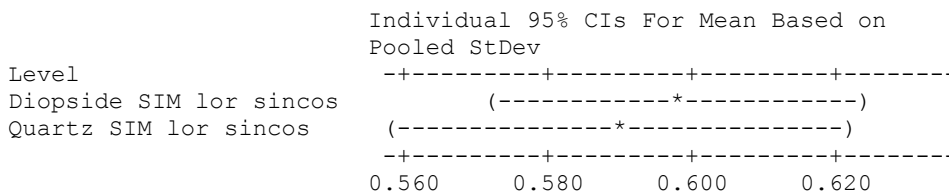
Pooled StDev = 0.04125

**One-way ANOVA: Diopside SIM lor sincos, Quartz SIM lor sincos**

Source	DF	SS	MS	F	P
Factor	1	0.00025	0.00025	0.16	0.694
Error	15	0.02369	0.00158		
Total	16	0.02395			

S = 0.03974    R-Sq = 1.06%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Diopside SIM lor sincos	10	0.59780	0.05123
Quartz SIM lor sincos	7	0.58994	0.00354



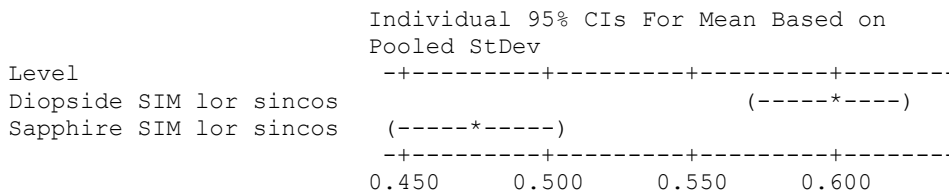
Pooled StDev = 0.03974

**One-way ANOVA: Diopside SIM lor sincos, Sapphire SIM lor sincos**

Source	DF	SS	MS	F	P
Factor	1	0.06610	0.06610	43.84	0.000
Error	16	0.02412	0.00151		
Total	17	0.09022			

S = 0.03883    R-Sq = 73.26%    R-Sq(adj) = 71.59%

Level	N	Mean	StDev
Diopside SIM lor sincos	10	0.59780	0.05123
Sapphire SIM lor sincos	8	0.47585	0.00847



Pooled StDev = 0.03883

**One-way ANOVA: Fluorapatite SIM lor sincos, Olivine SIM lor sincos**

Source	DF	SS	MS	F	P
Factor	1	0.022542	0.022542	176.06	0.000
Error	10	0.001280	0.000128		
Total	11	0.023822			

S = 0.01132    R-Sq = 94.63%    R-Sq(adj) = 94.09%



Level	N	Mean	StDev
Fluorapatite SIM lor sin	6	0.30577	0.01470
Olivine SIM lor sincos	6	0.39245	0.00632

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI Lower	CI Upper
Fluorapatite SIM lor sin	(---*--)	
Olivine SIM lor sincos		(---*--)

0.300      0.330      0.360      0.390

Pooled StDev = 0.01132

### One-way ANOVA: Fluorapatite SIM lor sincos, Quartz SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.260904	0.260904	2482.97	0.000
Error	11	0.001156	0.000105		
Total	12	0.262060			

S = 0.01025      R-Sq = 99.56%      R-Sq(adj) = 99.52%

Level	N	Mean	StDev
Fluorapatite SIM lor sin	6	0.30577	0.01470
Quartz SIM lor sincos	7	0.58994	0.00354

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI Lower	CI Upper
Fluorapatite SIM lor sin	(*)	
Quartz SIM lor sincos		(*)

0.320      0.400      0.480      0.560

Pooled StDev = 0.01025

### One-way ANOVA: Fluorapatite SIM lor sincos, Sapphire SIM lor sincos

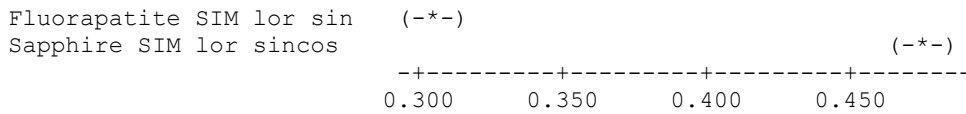
Source	DF	SS	MS	F	P
Factor	1	0.099183	0.099183	751.64	0.000
Error	12	0.001583	0.000132		
Total	13	0.100766			

S = 0.01149      R-Sq = 98.43%      R-Sq(adj) = 98.30%

Level	N	Mean	StDev
Fluorapatite SIM lor sin	6	0.30577	0.01470
Sapphire SIM lor sincos	8	0.47585	0.00847

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI Lower	CI Upper
	-+-----+-----+-----+-----	



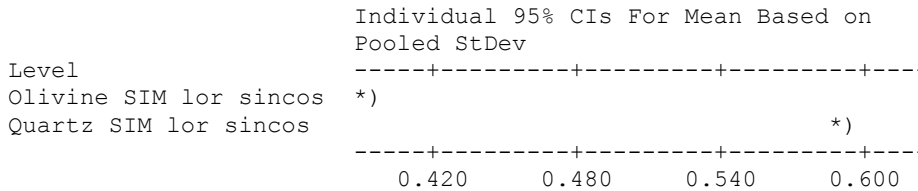
Pooled StDev = 0.01149

**One-way ANOVA: Olivine SIM lor sincos, Quartz SIM lor sincos**

Source	DF	SS	MS	F	P
Factor	1	0.1260111	0.1260111	5048.30	0.000
Error	11	0.0002746	0.0000250		
Total	12	0.1262856			

S = 0.004996 R-Sq = 99.78% R-Sq(adj) = 99.76%

Level	N	Mean	StDev
Olivine SIM lor sincos	6	0.39245	0.00632
Quartz SIM lor sincos	7	0.58994	0.00354



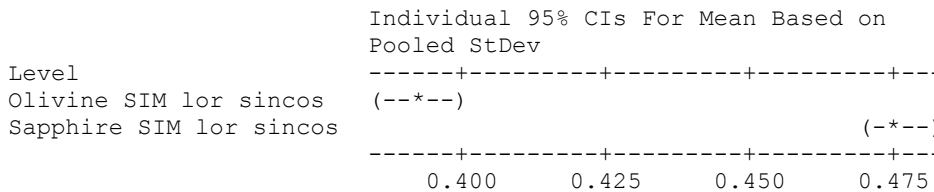
Pooled StDev = 0.00500

**One-way ANOVA: Olivine SIM lor sincos, Sapphire SIM lor sincos**

Source	DF	SS	MS	F	P
Factor	1	0.0238476	0.0238476	407.54	0.000
Error	12	0.0007022	0.0000585		
Total	13	0.0245498			

S = 0.007650 R-Sq = 97.14% R-Sq(adj) = 96.90%

Level	N	Mean	StDev
Olivine SIM lor sincos	6	0.39245	0.00632
Sapphire SIM lor sincos	8	0.47585	0.00847



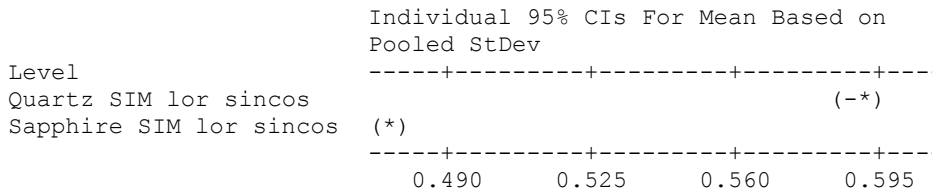
Pooled StDev = 0.00765

### One-way ANOVA: Quartz SIM lor sincos, Sapphire SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.0485975	0.0485975	1093.67	0.000
Error	13	0.0005777	0.0000444		
Total	14	0.0491751			

S = 0.006666 R-Sq = 98.83% R-Sq(adj) = 98.73%

Level	N	Mean	StDev
Quartz SIM lor sincos	7	0.58994	0.00354
Sapphire SIM lor sincos	8	0.47585	0.00847



Pooled StDev = 0.00667

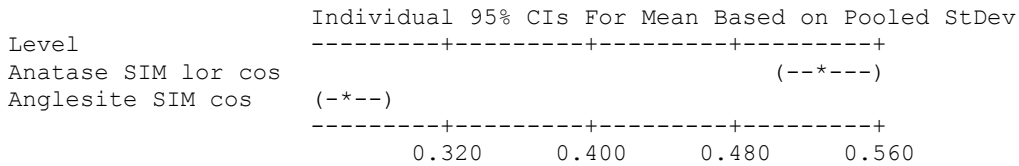
### Outlier removed

### One-way ANOVA: Anatase SIM lor cos, Anglesite SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.140220	0.140220	380.92	0.000
Error	7	0.002577	0.000368		
Total	8	0.142797			

S = 0.01919 R-Sq = 98.20% R-Sq(adj) = 97.94%

Level	N	Mean	StDev
Anatase SIM lor cos	3	0.53117	0.02595
Anglesite SIM cos	6	0.26638	0.01568



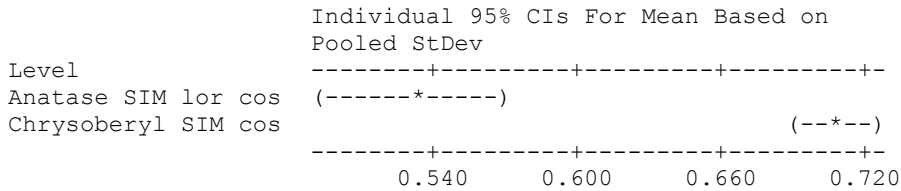
Pooled StDev = 0.01919

### One-way ANOVA: Anatase SIM lor cos, Chrysoberyl SIM cos

Source	DF	SS	MS	F	P
Factor	1	0.07594	0.07594	74.08	0.000
Error	15	0.01538	0.00103		
Total	16	0.09132			

S = 0.03202 R-Sq = 83.16% R-Sq(adj) = 82.04%

Level	N	Mean	StDev
Anatase SIM lor cos	3	0.53117	0.02595
Chrysoberyl SIM cos	14	0.70649	0.03285



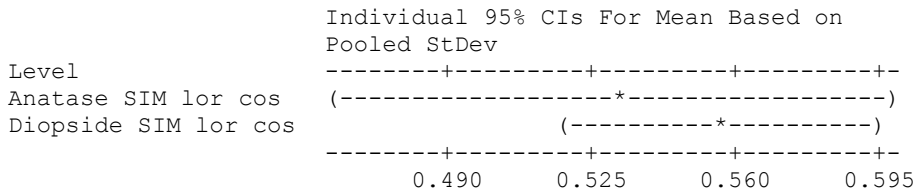
Pooled StDev = 0.03202

### One-way ANOVA: Anatase SIM lor cos, Diopside SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.00145	0.00145	0.50	0.494
Error	11	0.03182	0.00289		
Total	12	0.03326			

S = 0.05378    R-Sq = 4.35%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Anatase SIM lor cos	3	0.53117	0.02595
Diopside SIM lor cos	10	0.55621	0.05819



Pooled StDev = 0.05378

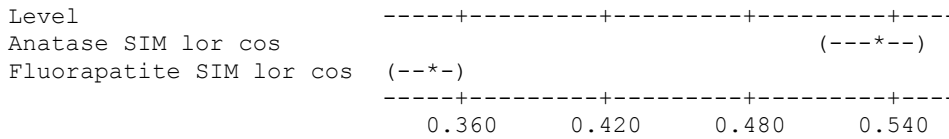
### One-way ANOVA: Anatase SIM lor cos, Fluorapatite SIM lor cos

Source	DF	SS	MS	F	P
Factor	1	0.067271	0.067271	275.31	0.000
Error	7	0.001710	0.000244		
Total	8	0.068982			

S = 0.01563    R-Sq = 97.52%    R-Sq(adj) = 97.17%

Level	N	Mean	StDev
Anatase SIM lor cos	3	0.53117	0.02595
Fluorapatite SIM lor cos	6	0.34777	0.00853

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.01563

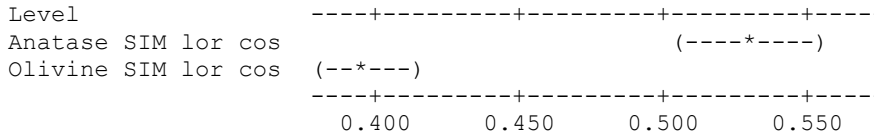
**One-way ANOVA: Anatase SIM lor cos, Olivine SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.036423	0.036423	113.20	0.000
Error	7	0.002252	0.000322		
Total	8	0.038675			

S = 0.01794    R-Sq = 94.18%    R-Sq(adj) = 93.34%

Level	N	Mean	StDev
Anatase SIM lor cos	3	0.53117	0.02595
Olivine SIM lor cos	6	0.39622	0.01346

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.01794

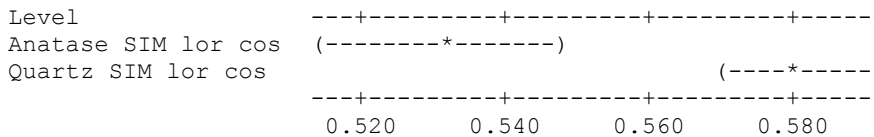
**One-way ANOVA: Anatase SIM lor cos, Quartz SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.005194	0.005194	29.41	0.001
Error	8	0.001413	0.000177		
Total	9	0.006607			

S = 0.01329    R-Sq = 78.62%    R-Sq(adj) = 75.94%

Level	N	Mean	StDev
Anatase SIM lor cos	3	0.53117	0.02595
Quartz SIM lor cos	7	0.58090	0.00332

Individual 95% CIs For Mean Based on Pooled StDev



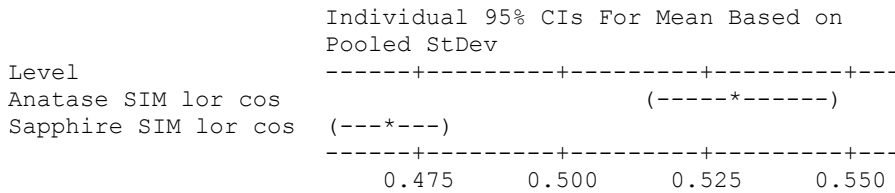
Pooled StDev = 0.01329

**One-way ANOVA: Anatase SIM lor cos, Sapphire SIM lor cos**

Source	DF	SS	MS	F	P
Factor	1	0.008257	0.008257	48.74	0.000
Error	9	0.001525	0.000169		
Total	10	0.009781			

S = 0.01302    R-Sq = 84.41%    R-Sq(adj) = 82.68%

Level	N	Mean	StDev
Anatase SIM lor cos	3	0.53117	0.02595
Sapphire SIM lor cos	8	0.46965	0.00504



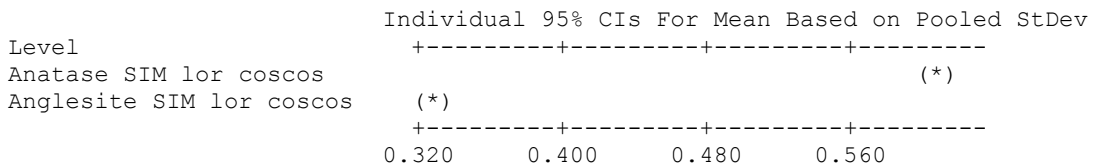
Pooled StDev = 0.01302

**One-way ANOVA: Anatase SIM lor coscos, Anglesite SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.1535688	0.1535688	3510.95	0.000
Error	7	0.0003062	0.0000437		
Total	8	0.1538750			

S = 0.006614    R-Sq = 99.80%    R-Sq(adj) = 99.77%

Level	N	Mean	StDev
Anatase SIM lor coscos	3	0.60557	0.01198
Anglesite SIM lor coscos	6	0.32847	0.00195



Pooled StDev = 0.00661

**One-way ANOVA: Anatase SIM lor coscos, Chrysoberyl SIM lor coscos**

Source	DF	SS	MS	F	P
Factor	1	0.078326	0.078326	90.12	0.000
Error	15	0.013037	0.000869		
Total	16	0.091363			

S = 0.02948    R-Sq = 85.73%    R-Sq(adj) = 84.78%

Level	N	Mean	StDev
Anatase SIM lor coscos	3	0.60557	0.01198
Chrysoberyl SIM lor cosc	14	0.78362	0.03132

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anatase SIM lor coscos	(-----*-----)
Chrysoberyl SIM lor cosc	(--*--)

0.600      0.660      0.720      0.780

Pooled StDev = 0.02948

### One-way ANOVA: Anatase SIM lor coscos, Diopside SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.00158	0.00158	0.25	0.627
Error	11	0.06939	0.00631		
Total	12	0.07097			

S = 0.07943    R-Sq = 2.22%    R-Sq(adj) = 0.00%

Level	N	Mean	StDev
Anatase SIM lor coscos	3	0.60557	0.01198
Diopside SIM lor coscos	10	0.63170	0.08763

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anatase SIM lor coscos	(-----*-----)
Diopside SIM lor coscos	(-----*-----)

0.540      0.600      0.660      0.720

Pooled StDev = 0.07943

### One-way ANOVA: Anatase SIM lor coscos, Fluorapatite SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.00521	0.00521	2.81	0.138
Error	7	0.01300	0.00186		
Total	8	0.01821			

S = 0.04310    R-Sq = 28.62%    R-Sq(adj) = 18.42%

Level	N	Mean	StDev
Anatase SIM lor coscos	3	0.60557	0.01198
Fluorapatite SIM lor cos	6	0.55452	0.05043

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anatase SIM lor coscos	(-----*-----)
Fluorapatite SIM lor cos	(-----*-----)

0.520      0.560      0.600      0.640

Pooled StDev = 0.04310

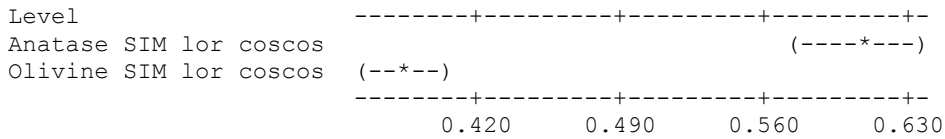
### One-way ANOVA: Anatase SIM lor coscos, Olivine SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.098701	0.098701	224.53	0.000
Error	7	0.003077	0.000440		
Total	8	0.101778			

S = 0.02097 R-Sq = 96.98% R-Sq(adj) = 96.54%

Level	N	Mean	StDev
Anatase SIM lor coscos	3	0.60557	0.01198
Olivine SIM lor coscos	6	0.38342	0.02362

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.02097

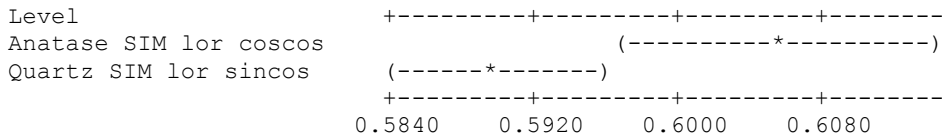
### One-way ANOVA: Anatase SIM lor coscos, Quartz SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.0005126	0.0005126	11.32	0.010
Error	8	0.0003622	0.0000453		
Total	9	0.0008748			

S = 0.006728 R-Sq = 58.60% R-Sq(adj) = 53.42%

Level	N	Mean	StDev
Anatase SIM lor coscos	3	0.60557	0.01198
Quartz SIM lor sincos	7	0.58994	0.00354

Individual 95% CIs For Mean Based on Pooled StDev



Pooled StDev = 0.00673

### One-way ANOVA: Anatase SIM lor coscos, Sapphire SIM lor coscos

Source	DF	SS	MS	F	P
Factor	1	0.0048231	0.0048231	78.71	0.000
Error	9	0.0005515	0.0000613		
Total	10	0.0053746			

S = 0.007828 R-Sq = 89.74% R-Sq(adj) = 88.60%



Level	N	Mean	StDev
Anatase SIM lor coscos	3	0.60557	0.01198
Sapphire SIM lor coscos	8	0.55855	0.00615

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Anatase SIM lor coscos	(---*---)	(-----*-----)
Sapphire SIM lor coscos	(---*---)	(---*---)

0.560      0.576      0.592      0.608

Pooled StDev = 0.00783

### One-way ANOVA: Anatase SIM lor sincos, Anglesite SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.336856	0.336856	544.71	0.000
Error	7	0.004329	0.000618		
Total	8	0.341185			

S = 0.02487      R-Sq = 98.73%      R-Sq(adj) = 98.55%

Level	N	Mean	StDev
Anatase SIM lor sincos	3	0.56110	0.02825
Anglesite SIM lor sincos	6	0.15070	0.02338

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Anatase SIM lor sincos	(---*---)	(---*---)
Anglesite SIM lor sincos	(-*)	(-*)

0.24      0.36      0.48      0.60

Pooled StDev = 0.02487

### One-way ANOVA: Anatase SIM lor sincos, Chrysoberyl SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.110425	0.110425	227.00	0.000
Error	15	0.007297	0.000486		
Total	16	0.117722			

S = 0.02206      R-Sq = 93.80%      R-Sq(adj) = 93.39%

Level	N	Mean	StDev
Anatase SIM lor sincos	3	0.56110	0.02825
Chrysoberyl SIM lor sinc	14	0.77251	0.02094

Individual 95% CIs For Mean Based on Pooled StDev

Level	Lower CI	Upper CI
Anatase SIM lor sincos	(---*---)	(---*---)
Chrysoberyl SIM lor sinc	(---*---)	(*---)

0.560      0.630      0.700      0.770

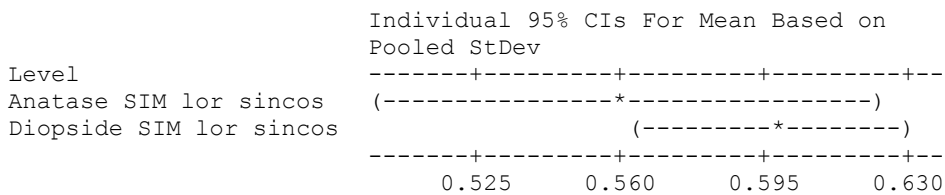
Pooled StDev = 0.02206

### One-way ANOVA: Anatase SIM lor sincos, Diopside SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.00311	0.00311	1.36	0.269
Error	11	0.02521	0.00229		
Total	12	0.02832			

S = 0.04788 R-Sq = 10.97% R-Sq(adj) = 2.88%

Level	N	Mean	StDev
Anatase SIM lor sincos	3	0.56110	0.02825
Diopside SIM lor sincos	10	0.59780	0.05123



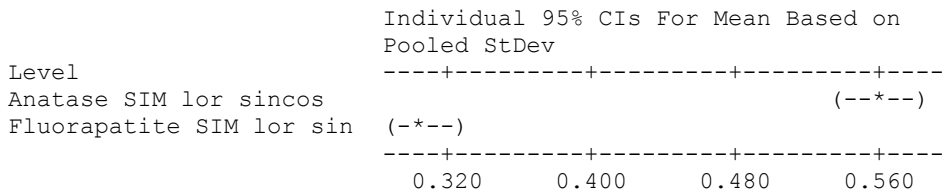
Pooled StDev = 0.04788

### One-way ANOVA: Anatase SIM lor sincos, Fluorapatite SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.130390	0.130390	340.90	0.000
Error	7	0.002677	0.000382		
Total	8	0.133068			

S = 0.01956 R-Sq = 97.99% R-Sq(adj) = 97.70%

Level	N	Mean	StDev
Anatase SIM lor sincos	3	0.56110	0.02825
Fluorapatite SIM lor sin	6	0.30577	0.01470



Pooled StDev = 0.01956

### One-way ANOVA: Anatase SIM lor sincos, Olivine SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.056886	0.056886	221.69	0.000
Error	7	0.001796	0.000257		
Total	8	0.058682			

S = 0.01602 R-Sq = 96.94% R-Sq(adj) = 96.50%

Level	N	Mean	StDev
Anatase SIM lor sincos	3	0.56110	0.02825
Olivine SIM lor sincos	6	0.39245	0.00632

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anatase SIM lor sincos	(---*--)
Olivine SIM lor sincos	(-*--)

0.420      0.480      0.540      0.600

Pooled StDev = 0.01602

### One-way ANOVA: Anatase SIM lor sincos, Quartz SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.001747	0.001747	8.36	0.020
Error	8	0.001672	0.000209		
Total	9	0.003419			

S = 0.01446    R-Sq = 51.10%    R-Sq(adj) = 44.99%

Level	N	Mean	StDev
Anatase SIM lor sincos	3	0.56110	0.02825
Quartz SIM lor sincos	7	0.58994	0.00354

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anatase SIM lor sincos	(-----*-----)
Quartz SIM lor sincos	(-----*-----)

0.544      0.560      0.576      0.592

Pooled StDev = 0.01446

### One-way ANOVA: Anatase SIM lor sincos, Sapphire SIM lor sincos

Source	DF	SS	MS	F	P
Factor	1	0.015857	0.015857	67.98	0.000
Error	9	0.002099	0.000233		
Total	10	0.017956			

S = 0.01527    R-Sq = 88.31%    R-Sq(adj) = 87.01%

Level	N	Mean	StDev
Anatase SIM lor sincos	3	0.56110	0.02825
Sapphire SIM lor sincos	8	0.47585	0.00847

Individual 95% CIs For Mean Based on Pooled StDev

Level	CI
Anatase SIM lor sincos	(-----*-----)
Sapphire SIM lor sincos	(---*---)

0.480      0.510      0.540      0.570

Pooled StDev = 0.01527

## APPENDIX E:

**Table V. Euclidean Distance Results Table**

Euclidean distance results calculated from an average reference vector that was transformed to unit vector length.

#	Sample	Distance (A.U.)	#	Sample	Distance (A.U.)
1	Anatase 1	3.0028	35	Fluorapatite 1	2.8206
2	Anatase 2	3.4903	36	Fluorapatite 2	2.8233
3	Anatase 3	3.3189	37	Fluorapatite 3	3.1936
4	Anatase 4	3.3229	38	Fluorapatite 4	2.4235
			39	Fluorapatite 5	3.2203
5	Anglesite 5	3.4428	40	Fluorapatite 6	2.5143
6	Anglesite 6	3.4436			
7	Anglesite 7	3.4495	41	Olivine 1	3.6078
8	Anglesite 8	3.4311	42	Olivine 2	3.1783
9	Anglesite 9	3.4505	43	Olivine 3	3.4513
10	Anglesite 10	3.4282	44	Olivine 4	3.1827
			45	Olivine 5	3.2137
11	Chrysoberyl 1	3.9204	46	Olivine 6	3.2371
12	Chrysoberyl 2	3.5787			
13	Chrysoberyl 3	3.2639	47	Quartz 1	2.6374
14	Chrysoberyl 4	3.2069	48	Quartz 2	2.6305
15	Chrysoberyl 5	2.957	49	Quartz 3	2.6399
16	Chrysoberyl 6	3.8561	50	Quartz 4	2.6244
17	Chrysoberyl 7	2.7541	51	Quartz 5	2.623
18	Chrysoberyl 8	3.7716	52	Quartz 6	2.6103
19	Chrysoberyl 9	3.1494	53	Quartz 7	2.5932
20	Chrysoberyl 10	3.7716			
21	Chrysoberyl 11	3.5615	54	Corundum 1	2.7214
22	Chrysoberyl 12	3.4525	55	Corundum 2	2.4269
23	Chrysoberyl 13	3.0691	56	Corundum 3	2.6101
24	Chrysoberyl 14	2.957	57	Corundum 4	2.4605
			58	Corundum 5	2.4605
25	Diopside 1	2.9018	59	Corundum 6	2.5503
26	Diopside 2	2.712	60	Corundum 7	1.676
27	Diopside 3	2.4195	61	Corundum 8	2.954
28	Diopside 4	1.5686			
29	Diopside 5	1.6806			
30	Diopside 6	1.5297			
31	Diopside 7	1.3823			
32	Diopside 8	1.6142			
33	Diopside 9	1.8486			
34	Diopside 10	2.8814			

**APPENDIX F:**

**Table VI. Mahalanobis Distance Results Table**

Mahalanobis distance results calculated from data that has been transformed to unit vector length. Results are based on use of an average reference vector.

#	Sample	Distance (A.U.)	#	Sample	Distance (A.U.)
1	Anatase 1	5542	35	Fluorapatite 1	4890
2	Anatase 2	7487	36	Fluorapatite 2	4899
3	Anatase 3	6770	37	Fluorapatite 3	6269
4	Anatase 4	6786	38	Fluorapatite 4	3610
			39	Fluorapatite 5	6374
5	Anglesite 5	7285	40	Fluorapatite 6	3885
6	Anglesite 6	7289			
7	Anglesite 7	7314	41	Olivine 1	8000
8	Anglesite 8	7236	42	Olivine 2	6208
9	Anglesite 9	7318	43	Olivine 3	7321
10	Anglesite 10	7223	44	Olivine 4	6226
			45	Olivine 5	6348
11	Chrysoberyl 1	9447	46	Olivine 6	6440
12	Chrysoberyl 2	7872			
13	Chrysoberyl 3	6548	47	Quartz 1	4275
14	Chrysoberyl 4	6321	48	Quartz 2	4253
15	Chrysoberyl 5	5374	49	Quartz 3	4283
16	Chrysoberyl 6	9139	50	Quartz 4	4233
17	Chrysoberyl 7	4662	51	Quartz 5	4228
18	Chrysoberyl 8	8743	52	Quartz 6	4188
19	Chrysoberyl 9	6096	53	Quartz 7	4133
20	Chrysoberyl 10	8743			
21	Chrysoberyl 11	7796	54	Corundum 1	4552
22	Chrysoberyl 12	7326	55	Corundum 2	3620
23	Chrysoberyl 13	5789	56	Corundum 3	4187
24	Chrysoberyl 14	5374	57	Corundum 4	3721
			58	Corundum 5	3721
25	Diopside 1	5175	59	Corundum 6	3997
26	Diopside 2	4520	60	Corundum 7	1726
27	Diopside 3	3598	61	Corundum 8	5363
28	Diopside 4	1512			
29	Diopside 5	1736			
30	Diopside 6	1438			
31	Diopside 7	1174			
32	Diopside 8	1601			
33	Diopside 9	2100			
34	Diopside 10	5103			

## APPENDIX G:

**Table VII. Mahalanobis Distance Results Table**

Mahalanobis distance results calculated from data that has been transformed to unit vector length. Results are based on statistical group mean and variance.

#	Sample	Mineral Group 1	Mineral Group 2	Mineral Group 3	Mineral Group 4	Mineral Group 5	Mineral Group 6	Mineral Group 7	Mineral Group 8
1	Anatase 1	491.89	2638.9	1892.1	3827.5	3146.6	2633.3	1767	2498.9
2	Anatase 2	77.908	3010.8	2179.4	4721.6	3765.4	3005.5	2386.7	3253.5
3	Anatase 3	576.73	2491.3	2246.7	3965.3	3154.2	2545.6	2476.9	3155.1
4	Anatase 4	25.964	2810.7	2109.3	4322.6	3492	2795	2282.7	3051.6
5	Anglesite 5	2632.8	0.41107	2580.4	4529.4	3240	2665.9	2593.9	3401.7
6	Anglesite 6	2631.8	0.63835	2578.5	4534.9	3243.3	2666.2	2597.5	3406.3
7	Anglesite 7	2605.8	1.2967	2591.6	4540.9	3244.7	2668.3	2598.2	3423.9
8	Anglesite 8	2602.1	1.5791	2563.9	4510.4	3243.7	2666.5	2596.7	3381.6
9	Anglesite 9	2600.9	1.576	2594.1	4541.3	3246.8	2669.1	2598.1	3424.8
10	Anglesite 10	2589.3	1.7794	2560.8	4507.5	3242.8	2665.9	2595.4	3380
11	Chrysoberyl 1	3975.9	4751.3	179.81	6688.7	5833.4	4190.4	3343	5021.3
12	Chrysoberyl 2	3527.2	4338	222.08	5604.9	5357.7	3968.1	2401.4	4869.7
13	Chrysoberyl 3	3166.1	3935.2	265.6	4745.7	4844.9	3575.8	2075.6	4305.3
14	Chrysoberyl 4	3164.6	3780.5	197.21	4699.4	4571.8	3410.2	2554	3978.7
15	Chrysoberyl 5	2913.1	3620.7	100.4	4381.6	4337.4	3234.1	2226.7	3582.1
16	Chrysoberyl 6	3914.9	4720.4	151.29	6606.5	5704.4	4020.5	3182.6	5177.6
17	Chrysoberyl 7	2265.7	3179.7	413.69	4095.4	3476.5	2626	1925.2	3764.9
18	Chrysoberyl 8	3775.3	4588.3	237.79	6236.1	5695.6	4066.6	2935.7	4915.2
19	Chrysoberyl 9	2836.3	3716.4	329.66	4923.2	4230	3135.8	2034.6	4428.1
20	Chrysoberyl 10	3775.3	4588.3	237.79	6236.1	5695.6	4066.6	2935.7	4915.2
21	Chrysoberyl 11	3312	4308.7	225.62	5759.7	5145.8	3626.3	2767	4820.7
22	Chrysoberyl 12	3405.5	4252	109.28	5476.3	5157.7	3750.2	2283.8	4837.2
23	Chrysoberyl 13	2666.9	3495.3	459.13	4658.4	3962.9	3062.1	1860.1	4364.3
24	Chrysoberyl 14	2913.1	3620.7	100.4	4381.6	4337.4	3234.1	2226.7	3582.1
25	Diopside 1	2369.3	2724.6	1631.9	503.06	3282.9	2574.7	2115.1	3229.7
26	Diopside 2	2262.9	2781.3	1402.2	745.59	3344.7	2644.2	1660.8	3070.2
27	Diopside 3	2060.1	2500	1263	587.31	2990.8	2383	1457.5	2858.7
28	Diopside 4	1406.3	1556.9	1384.4	198.19	1647.2	1544.6	1198	1603.1
29	Diopside 5	1439.1	1553.6	1461.2	232.15	1646.1	1541.4	1318.3	1620.7
30	Diopside 6	1342.5	1467.5	1439.3	348	1523.7	1478.7	1149.1	1483.1
31	Diopside 7	1299.2	1428.4	1371.8	444.28	1409.1	1433.9	1097.8	1339.4
32	Diopside 8	1393.2	1531.8	1448.9	275.59	1543.3	1513	1298	1517.1
33	Diopside 9	1655.9	2062.1	1227.2	299.23	2348.8	1979.1	1157.1	1787.1
34	Diopside 10	2384	2768.2	1581.8	750.52	3333.2	2614.2	2081	3125.2

35	<b>Fluorapatite 1</b>	2118.2	2161.8	2029.1	3386	10.339	1988.4	2094	2717.5
36	<b>Fluorapatite 2</b>	2122.9	2182.7	2028.3	3375.2	14.307	1987.9	2098.2	2718.4
37	<b>Fluorapatite 3</b>	2473.1	2512.3	2215.4	4057.5	86.221	2258.8	2483.1	3136
38	<b>Fluorapatite 4</b>	1825.1	1831.3	1886.9	2647.2	95.362	1701	1814.6	2119.7
39	<b>Fluorapatite 5</b>	2493.5	2547.7	2223.8	4121	101	2289.5	2491.4	3189.1
40	<b>Fluorapatite 6</b>	1895	1923.3	1907.3	2820.6	47.427	1755	1890.2	2255.1
41	<b>Olivine 1</b>	2921	2972.9	2419.9	5100.4	3547	22.897	2946	3950.2
42	<b>Olivine 2</b>	2492.1	2553.2	2162.7	4131.8	2891.9	245.87	2509.7	3254.7
43	<b>Olivine 3</b>	2801	2850.3	2309	4819.4	3129.6	37.052	2825.1	3736.4
44	<b>Olivine 4</b>	2544.2	2584.4	2168.5	4218.5	2796.5	9.7577	2560	3335.8
45	<b>Olivine 5</b>	2571.4	2629.6	2183.2	4309	2805	18.362	2597.3	3353.7
46	<b>Olivine 6</b>	2549.2	2584.9	2294.6	4104.7	2824.6	50.668	2567.5	3360
47	<b>Quartz 1</b>	2072.9	2555.1	1478.2	3093.7	3124.1	2598	1.4803	2961.4
48	<b>Quartz 2</b>	2073.5	2571.5	1462.3	3101.8	3142.6	2597.4	1.4144	2931.2
49	<b>Quartz 3</b>	2102.7	2579.9	1447.9	3126.4	3160.3	2625.4	15.336	2949.7
50	<b>Quartz 4</b>	2090.2	2566.6	1445.4	3099.2	3142	2617	15.067	2910.8
51	<b>Quartz 5</b>	2023.1	2539.7	1498	3050.6	3100	2588.5	8.4029	2883.1
52	<b>Quartz 6</b>	2011.8	2533.3	1493	3038	3090.8	2576.5	8.3401	2853.4
53	<b>Quartz 7</b>	2007.8	2532.1	1473.6	3018.5	3083.3	2557.4	8.5502	2850.4
54	<b>Corundum 1</b>	1897	2359.8	1772.5	3478.5	2830	2386.3	2066.9	72.654
55	<b>Corundum 2</b>	1704.2	2118	1681.5	2922.3	2469.8	2142.8	1816.2	8.8508
56	<b>Corundum 3</b>	1804.8	2265.2	1781.6	3089.2	2660.1	2256.8	1955	123.08
57	<b>Corundum 4</b>	1734.3	2137.8	1677.5	2989.5	2516.4	2174.3	1863.9	42.303
58	<b>Corundum 5</b>	1734.3	2137.8	1677.5	2989.5	2516.4	2174.3	1863.9	42.303
59	<b>Corundum 6</b>	1810.8	2225	1698.1	3158.7	2643.3	2259.2	1913.4	38.056
60	<b>Corundum 7</b>	1248.5	1384.6	1607.6	1451.4	1429.7	1439.2	1288.8	674.1
61	<b>Corundum 8</b>	2121.6	2593.6	1846	3842.1	3180.4	2598.7	2255.1	220.98

## APPENDIX H:

### SIM Calibration Matlab Program dbcalcsv3f.m

```
%This code performs background subtraction and calibration of the Raman
%spectra in the mineral database and prepares PHP database lists for
%uploading information
% Start Date: 9/20/2010
% Author: Robert Cannon
%
% This code operates on the following variables: dspemat rawspemat
bgspemat penspemat.
% These variables are loaded into memory from *.mat files of the same
name
%
% Code Porting Information: penref_path needs to be hardwired to the
correct directory if code is ported to another PC

clear
close all

%This code builds on the work of Dr.John F. Turner II, Jon Damsel and
%Nick Neric

% Open Error Log File for writing
% if exist('c:\c1\raman_mindb','dir')~=7
%     if exist('c:\c1')~=7
%         cd('c:');
%         mkdir('c1');
%     end
%     cd('c:\c1')
%     mkdir('raman_mindb');
% end

errorfid=fopen('c:\c1\raman_mindb\mindb_error.rtf','a');

%Open Error Log File for writing
if
exist('c:\Users\Antoinette\Desktop\RC\Gradwork\raman_mindb','dir')~=7
    if exist('c:\Users\Antoinette\Desktop\RC\Gradwork')~=7
        cd('c:');
        mkdir('\Antoinette\Desktop\RC\Gradwork');
    end
    cd('c:\\Antoinette\Desktop\RC\Gradwork')
    mkdir('raman_mindb');
end

errorfid=fopen('c:\Users\Antoinette\Desktop\RC\Gradwork\raman_mindb\min
db_error.txt','a');

seeplots=1;                % Change value to 1 in order to see the plots
skipflag=0;
sim_thresh=.85;           % was .85
```



```

neighborhood=11;          % a hard-wired value that may need changed--
must be an odd number (was 11,7)
fwhm=9;                  % a hard-wired value that may need changed--
This number establishes the width of the lorentzian (9)
shiftlog=[0 0];

firstindex=ceil(neighborhood/2);

penref_path='C:\Users\Antoinette\Desktop\RC\Gradwork\good\';
%penref_path='C:\C1\RobertCannon\dbc calibrate\good\';%Penlamp reference
files  TODO: Change this path to the generic path for the dbmin
database
if exist(penref_path,'dir')~=7
    [filename,penref_path]=uigetfile('*.','Select Penlamp Reference
File Directory');
end

>Delete: penref_path='C:\Users\Antoinette\Desktop\RC\Gradwork\good\';

% Load (data) path and datafile matrices with rf10_20_092 & pb_next;

rf10_20_092; %Sort out the good directories; Old file usedrf10_20_092;
pb_next; %Condensed call for the code below

%load C:\Users\Antoinette\Desktop\RC\Gradwork\dspemath.mat dspemath;
%load C:\Users\Antoinette\Desktop\RC\Gradwork\rawspemat.mat rawspemat;
%load C:\Users\Antoinette\Desktop\RC\Gradwork\bgspemat.mat bgspemat;
%load C:\Users\Antoinette\Desktop\RC\Gradwork\penspemat.mat penspemat;

%load C:\C1\RobertCannon\dbc calibrate\dspemath.mat dspemath;%Delete:
%load C:\C1\RobertCannon\dbc calibrate\rawspemat.mat rawspemat;%Delete:
%load C:\C1\RobertCannon\dbc calibrate\bgspemat.mat bgspemat;%Delete:
%load C:\C1\RobertCannon\dbc calibrate\penspemat.mat penspemat;%Delete:

if
exist('dspemath','var')&exist('rawspemat','var')&exist('bgspemat','var'
)&exist('penspemat','var')~=1

%TODO: This error checking should be done in Jon's Code and then this
can be deleted.
    error('The following variables are not loaded: dspemath, rawspemat,
bgspemat, penspemat');
end

% open raw and background files, perform background subtraction, open
penlamp file, perform calibration and save calibrated file. Also save
a filedescripto that include intial path information and ???
z=1;
datadimension='uint16';
headersize=4100;
for dline=1:1:length(dspemath(:,1))

%only 242 for partial mindb file testing
dline=1:1:length(dspemath(1:242,1))

```

```

dline
skipflag=0;
saveflag=1;

%Spectrum data set count
for triplet=1:1:3

    if triplet==1 %penlamp spectrum
        namepath=strcat(dspemath(dline,:), penspemat(dline,:));
        if isempty(findstr(penspemat(dline,:), '_532nm_')==0

% Change to findstr is valid for Matlab 5.3
            laser=532;
            laserstr='_532nm_';
        elseif isempty(findstr(penspemat(dline,:), '_785nm_')==0
            laser=785;
            laserstr='_785nm_';
        else
            laser=0;
        end

        if isempty(findstr(penspemat(dline,:), '_1500dcm')==0
            dcm=1500;
            dcmstr='_1500dcm_';
        elseif isempty(findstr(penspemat(dline,:), '_1000dcm')==0
            dcm=1000;
            dcmstr='_1000dcm_';
        elseif isempty(findstr(penspemat(dline,:), '_500dcm')==0
            dcm=1000;
            dcmstr='_500dcm_';
        else
            dcm=0;
        end

        if isempty(findstr(penspemat(dline,:), 'neon')==0
            pentype='neon';
        elseif isempty(findstr(penspemat(dline,:), 'xenon')==0
            pentype='xenon';
        else
            pentype='none';
        end

    elseif triplet==2 %raw spectrum
        namepath=strcat(dspemath(dline,:), rawspemat(dline,:));
        namepathstr=namepath;
        slashes_ind=findstr(namepathstr, '\\');
        for slash=1:1:length(slashes_ind)
            namepathstr=[namepathstr(1,1:slashes_ind(slash)) ' '
namepathstr(1,slashes_ind(slash)+1:length(namepathstr(1,:)))]];
        namepathstr(1,slashes_ind(slash):slashes_ind(slash)+1)=='\\';
        slashes_ind=slashes_ind+1;
        end
        if
            isempty(findstr(rawspemat(dline,:), laserstr))==1 | isempty(findstr(rawspe
mat(dline,:), dcmstr))==1

```

```

        errorstr1=[namepathstr '\n'];
        errorstr2=['The laser and or wavenumber value in the
penlamp filename does not match the the rawspemat name (dline='
num2str(dline) ')\n\trawspemat:' rawspemat(dline,:) '\n\tpen Laser='
laserstr ' and pen wavenumber=' dcmstr '\n\n'];
        fprintf(errorfid,errorstr1);
        fprintf(errorfid,errorstr2);
        skipflag=1;
    end

elseif triplet==3 %background spectrum
    namepath=strcat(dspemath(dline,:), bgspemat(dline,:));
    namepathstr=namepath;
    slashes_ind=findstr(namepathstr,'\');
    for slash=1:1:length(slashes_ind)
        namepathstr=[namepathstr(1,1:slashes_ind(slash)) ' '
namepathstr(1,slashes_ind(slash)+1:length(namepathstr(1,:)))];
    namepathstr(1,slashes_ind(slash):slashes_ind(slash)+1)=='\';
        slashes_ind=slashes_ind+1;
    end
    if
isempty(findstr(bgspemat(dline,:),laserstr))==1|isempty(findstr(bgspema
t(dline,:),dcmstr))==1
        errorstr1=[namepathstr '\n'];
        errorstr2=['The laser and or wavenumber value in the
penlamp filename does not match the the bgspemat name (dline='
num2str(dline) ')\n\tbgspemat:' bgspemat(dline,:) '\n\tpen Laser='
laserstr ' and pen wavenumber=' dcmstr '\n\n'];
        fprintf(errorfid,errorstr1);
        fprintf(errorfid,errorstr2);
        skipflag=1;
    end
end

if skipflag==0
    fid=fopen(namepath,'r');

    sidata_pt=fseek(fid,42,'bof');
    x=fread(fid,[1,1],'int16');

    sidata_pt=fseek(fid,656,'bof');
    y=fread(fid,[1,1],'int16');

    sidata_pt=fseek(fid,1446,'bof');
    num_frames=fread(fid,[1,1],'int32');

    img_size=x*y;
    sizecoef=1000/(2*x); %for image transferring
    sidata_pt=fseek(fid,headersize,'bof');
    if triplet==1
        if exist('sidata')==1
            clear sidata;
        end
        sidata=fread(fid,[img_size,num_frames],datadimension);
    end
end

```

```

else
sidata_tmp=fread(fid,[img_size,num_frames],datadimension);
%Appends the raw and background in sidata
    sidata=[sidata sidata_tmp];
    clear sidata_tmp;
end
    fclose(fid);
end
end

if skipflag==0
    % Now perform calibration
    if strcmpi(pentype,'neon')&laser==532&dcm==1500
        penname='neonpen_532nm_1500dcm.mat';
        load([penref_path penname]);
        laserwavenum=1/(532*10^(-7));
        pencase=1;
    elseif strcmpi(pentype,'neon')&laser==785&dcm==1000
        penname='neonpen_785nm_1000dcm.mat';
        load([penref_path penname]);
        laserwavenum=1/(784.74*10^(-7));
        pencase=2;
    elseif strcmpi(pentype,'xenon')&laser==532&dcm==1500
        penname='xenonpen_532nm_1500dcm.mat';
        load([penref_path penname]);
        laserwavenum=1/(532*10^(-7));
        pencase=3;
    elseif strcmpi(pentype,'xenon')&laser==532&dcm==1000
        penname='xenonpen_532nm_1000dcm.mat';
        load([penref_path penname]);
        laserwavenum=1/(532*10^(-7));
        pencase=4;
    elseif strcmpi(pentype,'neon')&laser==785&dcm==500
        penname='neonpen_785nm_500dcm.mat';
        load([penref_path penname]);
        laserwavenum=1/(784.74*10^(-7));
        pencase=5;
    else
        fprintf('There is no reference penlamp spectrum for this
case');
        break;
    end

    if pencase==1

refpeakmat=[101,540.0562;778,585.2488;916,594.4834;1144,609.6163;1214,6
14.3063;1245,616.3594;1326,621.7281];
        elseif pencase==2
            refpeakmat=[25,
808.2458;106,813.6406;352,830.0326;469,837.7606;647,849.5360;888,865.43
83;1208,885.3867];
        elseif pencase==3
            refpeakmat=[573, 571.610;812,587.502;898,593.417];
        elseif pencase==4

```

```

        refpeakmat=[574, 571.610;813,587.502;900,593.417];
elseif pencase==5

refpeakmat=[545,808.2458;626,813.6406;873,830.0326;990,837.7606;1168,84
9.5360];

end

spec=[sidata(:,1) penref]; %Appended penref to try to save
writing extra code

%plot(spec(:,1)); %return plots
%plot(spec(:,2))
%plot(sidata(:,2))
%plot(sidata(:,3))

%caldata_xmat can be change to a desired range
caldata_x=1:1340;
caldata_x=caldata_x';
caldata_xmat=caldata_x;

numspec=length(spec(1,:));

if numspec>=2;

    for g=2:1:numspec
        caldata_xmat=[caldata_xmat, caldata_x];% Dimensions all
x ranges for sidata
    end

    minspec=min(spec);
    maxspec=max(spec);
    specrange=maxspec-minspec;
    for k=1:1:length(spec(1,:)) %Normalizes all the spectra
        spec(:,k)=spec(:,k)-minspec(1,k);
        spec(:,k)=spec(:,k)./specrange(1,k);
    end

end

%This spectra is smoothed and a threshlod level is calculated here
vect_lormat=zeros(length(spec(:,1)),length(spec(1,:)));
for s=1:1:length(spec(1,:))
    %Medfilt2 is used to smooth out the data
    specsmoothed=medfilt2(spec(:,s),[6 1]);
    %first: calculate noise so that signal level that
corresponds to s/n=2 is known
    smoorawdiff=abs(spec(:,s)-specsmoothed);
    newsmoorawdiff=zeros(neighborhood,length(smoorawdiff(:,1))-
neighborhood+1); %Makes the spectral shift
    for j=1:1:neighborhood % this loop makes a matrix of data
that is similar in meaning to an image data set, but the spectra
correspond to neighborhood values

```

```

newsmoorawdiff(j,:)=smoorawdiff(j:length(smoorawdiff(:,1))-
neighborhood+j,1)'; %Need to calculate the noise
    end
    minnewsmoorawdiff=min(newsmoorawdiff);
    [min_minnewsmoorawdiff
sidata_noiseindex]=min(minnewsmoorawdiff);

noise=std(spec(sidata_noiseindex:sidata_noiseindex+neighborhood-1,s)-
specsmoothed(sidata_noiseindex:sidata_noiseindex+neighborhood-1,1));
%Used to find threshold

    %%%%finding lowest sim_thresh for all spec%%%%%%%%%
    % generating a lorentzian reference vector shaped as
closely to what we want for the noise?
    ref_vect_lor_noiz = zeros(1,neighborhood);
    for i = 1:1:neighborhood
        ref_vect_lor_noiz(1,i) = 2*noise*((fwhm)^2)/(fwhm.^2 +
(i-firstindex)^2);
        %ref_vect_lor_noiz(1,i) = (2*noise)/(1+((i-
firstindex)/fwhm)^2);
    end
    %%Calculate sin and cos perturbation functions for noise
estimations
    cospertfun=zeros(length(ref_vect_lor_noiz(1,:)),1);
    sinpertfun=zeros(length(ref_vect_lor_noiz(1,:)),1);
    count=1;
    for angle=0:2*pi/length(ref_vect_lor_noiz(1,:)):2*pi
        cospertfun(count,1)=cos(angle);
        sinpertfun(count,1)=sin(angle);
        count=count+1;
    end
    cosref_vect_lor_noiz=ref_vect_lor_noiz.*0;
    sinref_vect_lor_noiz=ref_vect_lor_noiz.*0;
    for j=1:1:length(ref_vect_lor_noiz(1,:))

cosref_vect_lor_noiz(1,j)=ref_vect_lor_noiz(1,j).*cospertfun(j,1)';
sinref_vect_lor_noiz(1,j)=ref_vect_lor_noiz(1,j).*sinpertfun(j,1)';
    end

    % CODE BLOCK A    % This block of code calculates the
lowest sim_thresh values for all perturbation cases.  Historically, the
product of these
    % values
(lowest_sim_thresh*lowest_cossim_thresh*lowest_sinsim_thresh) gives the
lowest SIM threshold score for a spectrum snippit that should be
identified as a peak.  Presently,
    % this code is not used anywhere else in this program as of
findpeaks20.  Parts of this block have been hardwired elsewhere-- in
the CCA section.
    %%%Using Geometry (Which geometric theorem?? Pythag?)
    %%%%for unperturbed

```

```

        l=2*noise*((neighborhood-1)^.5);%The 2 was added to improve
performance
        b=(sum(ref_vect_lor_noiz(1,:).^2))^0.5;
        lowest_sim_thresh=(1-(l^2/((neighborhood-1)*b^2)))^0.5;

        %%%%for cos perturbed %%Note: for cos and sin: Because
cos and sin are weighing functions and because they would integrate to
0.5 if increment was infinitesimally small- but they are not
        cos_l=(sum(l*cospertfun)/length(cospertfun(:,1)));% This is
true on average,but the noise is not uniformly distributed between
wavelengths like we do it here.
        cos_b=(sum(cosref_vect_lor_noiz(1,:).^2))^0.5;
        lowest_cossim_thresh=(1-(l^2/((neighborhood-1)*b^2)))^0.5;
        %%%%for sin perturbed
        sin_l=(sum(l*sinpertfun)/length(sinpertfun(:,1)));% This is
true on average, but the noise is not uniformly distributed between
wavelengths like we do it here.
        sin_b=(sum(sinref_vect_lor_noiz(1,:).^2))^0.5;
        lowest_sinsim_thresh=(1-(l^2/((neighborhood-1)*b^2)))^0.5;
%Found on line 384 for thresh_threshline
        %END CODE BLOCK A

        %Normalize specssmoothed to make nspecsmoothed % This is
done so that drawing in the peak lines is easier-- all are 1 unit high
        minspectsmoothed = min(specsmoothed); %This is the first
spectra, below are the shifted spectra
        maxspectsmoothed = max(specsmoothed);
        specrangesmoothed = maxspectsmoothed - minspectsmoothed ;
        nspectsmoothed= specsmoothed-minspectsmoothed;
        nspectsmoothed= nspectsmoothed./specrangesmoothed;

        % These are all the shifted spectra use matrix-based
sliding window (neighborhood) to find peaks. The
        % peak finding method is based on SIM.
        nspectsmoothed_mat=zeros(length(nspectsmoothed(:,1))-
neighborhood+1,neighborhood);
        for j=1:1:neighborhood % this loop makes a matrix of data
that is similar in meaning to an image data set, but the spectra are
shifted correspond to neighborhood values

nspectsmoothed_mat(:,j)=nspectsmoothed(j:length(nspectsmoothed(:,1))-
neighborhood+j,1);
        end

        nspectsmoothed_mat_temp=nspectsmoothed_mat; %just a copy of
newspec for comparison at the end

        %normalize newspec spectrally
        minnspectsmoothed_mat = min(nspectsmoothed_mat');
        maxnspectsmoothed_mat = max(nspectsmoothed_mat');
        specrangesmoothed = maxnspectsmoothed_mat -
minnspectsmoothed_mat;

        for j=1:1:neighborhood
            nspectsmoothed_mat(:,j)= nspectsmoothed_mat(:,j)-
minnspectsmoothed_mat';

```

```

        nspecsmoothed_mat(:,j)=
nspecsmoothed_mat(:,j)./specrangesmoothed';
    end

    %%Calculate sin and cos perturbation functions:
    cospertfun=zeros(length(nspecsmoothed_mat(1,:)),1);
    sinpertfun=zeros(length(nspecsmoothed_mat(1,:)),1);

    count=1;
    for angle=0:2*pi/length(nspecsmoothed_mat(1,:)):2*pi
        cospertfun(count,1)=cos(angle);
        sinpertfun(count,1)=sin(angle);
        count=count+1;
    end

    for j=1:1:length(nspecsmoothed_mat(1,:))
        cosspec(:,j)=nspecsmoothed_mat(:,j).*cospertfun(j,1);
        sinspec(:,j)=nspecsmoothed_mat(:,j).*sinpertfun(j,1);
    end%TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTtest--

    % now to normalize the cosspec and sinspec data sets across
    their column dimension
    mincosspec = min(cosspec');
    maxcosspec = max(cosspec');
    cosspecrange = maxcosspec - mincosspec;

    for j=1:1:neighborhood
        cosspec(:,j)= cosspec(:,j)-mincosspec';
    end

    %TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTEST
        %plot([cosspec(:,ceil(neighborhood/2))]); pause;

        cosspec(:,j)= cosspec(:,j)./cosspecrange';
    end

    minsinspec = min(sinspec');
    maxsinspec = max(sinspec');
    sinspecrange = maxsinspec - minsinspec;

    for j=1:1:neighborhood
        sinspec(:,j)= sinspec(:,j)-minsinspec';
        sinspec(:,j)= sinspec(:,j)./sinspecrange';
    end

    % generating a lorentzian reference vector shaped as
    closely to what we want
    %%Changed from Findpeaks 22, we now are able to search
    against different reference spectral shapes.
    %stand_dev=fwhm/((8*log(2))^1/2); %this is done because, we
    need standard deviation to calculate the gaussian curve

```



```

        stand_dev=(fwhm-1)/2.35482; %couldn't get the formula to
work, so I used its rounded value instead. Numbers are pretty close.
        %NOTE: I don't know why I need the (-1). Without it it,
FWHM turns out to be one too many

        ref_vect_lor = zeros(1,neighborhood);
        %default=menu(['Please choose the type of referece vector
you would like to find peaks
with:'],'Lorentzian','Gaussian','square','triangle','Voigt');
        %if default==1
        for i = 1:1:neighborhood %lorentzian
            ref_vect_lor(1,i) = ((fwhm)^2)/(fwhm.^2 + (i-
firstindex)^2);
            %ref_vect_lor(1,i) = (1)/(1+((i-firstindex)/fwhm)^2);
        end

        %end
        % generating the cos and sin perturbed lorentzian reference
vectors
        cosref_vect_lor=zeros(1,neighborhood);
        sinref_vect_lor=zeros(1,neighborhood);
        for j=1:1:length(nspectsmoothed_mat(1,:))

cosref_vect_lor(:,j)=ref_vect_lor(:,j).*cospertfun(j,1);

sinref_vect_lor(:,j)=ref_vect_lor(:,j).*sinpertfun(j,1);
        end

        %Delete rvl=(sum((ref_vect_lor.^2)'))^.5
        %Delete crvl=(sum((cosref_vect_lor.^2)'))^.5
        %Delete srvl=(sum((sinref_vect_lor.^2)'))^.5

        %Delete plot([ref_vect_lor' cosref_vect_lor'
sinref_vect_lor']);

        % normalizing ref_vect_lor, cosref_vect_lor, and
sinref_vect_lor
        ref_vect_lor=(ref_vect_lor-
min(ref_vect_lor))./(max(ref_vect_lor)-min(ref_vect_lor));
        cosref_vect_lor=(cosref_vect_lor-
min(cosref_vect_lor))./(max(cosref_vect_lor)-min(cosref_vect_lor));
        sinref_vect_lor=(sinref_vect_lor-
min(sinref_vect_lor))./(max(sinref_vect_lor)-min(sinref_vect_lor));

        %Delete plot([ref_vect_lor' cosref_vect_lor'
sinref_vect_lor']);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
        % The bit of code that follows is my way to make sure that
the length of all three reference vectors is exactly 1.

```

```

% By doing this, the cosine calculation is simplified
(hence the -1 and
% *1 in the numerator and denominator (For the CCA
calculation next)

for j=1:1:neighborhood
    clear tmp;
    clear costmp;
    clear sintmp;

    tmp=ref_vect_lor.^2;
    costmp=cosref_vect_lor.^2;
    sintmp=sinref_vect_lor.^2;

    tmp=(sum(tmp')).^0.5;
    costmp=(sum(costmp')).^0.5;
    sintmp=(sum(sintmp')).^0.5;

    ref_vect_lor=ref_vect_lor./tmp;
    cosref_vect_lor=cosref_vect_lor./costmp;
    sinref_vect_lor=sinref_vect_lor./sintmp;
end

clear tmp;
clear costmp;
clear sintmp;

rvl=(sum((ref_vect_lor.^2)'))^.5;
crvl=(sum((cosref_vect_lor.^2)'))^.5;
srvl=(sum((sinref_vect_lor.^2)'))^.5;

%Delete plot([ref_vect_lor' cosref_vect_lor'
sinref_vect_lor']);

%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%NOW DO C2=A2+B2-2ABcos(theta)% All data sets have
already been normalized.
%now perform CCA on spec
%_____Cosine
Correlation#####
#####

cosline=[zeros(1,length(nspecssmoothed_mat(:,1)))];
as_and_bs=0;

c_spec=[zeros(length(nspecssmoothed_mat(:,1)),neighborhood)];
c2_data=0;

as_and_bs=sum(nspecssmoothed_mat'.^2);
a_and_b=as_and_bs^(0.5); %Does this work because A or B is
equal to 1.

```

```

        for j=1:1:neighborhood
            c_spec(:,j)=nspecsmoothed_mat(:,j)-ref_vect_lor(1,j);
%Generates difference vectors
        end
        c2_data=sum(c_spec'.^2); %transposed
        %           for the length of the refence vector being 1^2, so
c2_data -1 - as_and_bs in the numerator.
        %           This is also why I wrote a redundant 1 in the
denominator-- commenting older code -jft2 1/19/2001

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

        cosline(1,:)=((c2_data)-1)-as_and_bs)./(-2*1.*a_and_b);
%Adjustment to theoretical 1 values for a & b
        %Delete plot(cosline);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%now perform CCA on cosspec
%           Cosine
Correlation#####
#####

        coscosline=[zeros(1,length(cosspec(:,1)))];
as_and_bs=0;
c_spec=[zeros(length(cosspec(:,1)),neighborhood)];
c2_data=0;

as_and_bs=sum(cosspec'.^2);
a_and_b=as_and_bs.^(0.5);

        for j=1:1:neighborhood
            c_spec(:,j)=cosspec(:,j)-cosref_vect_lor(1,j);
        end
        c2_data=sum(c_spec'.^2);
        %           for the length of the refence vector being 1^2, so
c2_data -1 - as_and_bs in the numerator.
        %           This is also why I wrote a redundant 1 in the
denominator-- commenting older code -jft2 1/19/2001

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

        coscosline(1,:)=((c2_data)-1)-as_and_bs)./(-2*1.*a_and_b);
%plot(coscosline);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%now perform CCA on sinspec
%           Cosine
Correlation#####
#####

        sincosline=[zeros(1,length(sinspec(:,1)))];
as_and_bs=0;

```



```

elseif
thresh_threshline(1,i)==1&i==length(thresh_threshline(1,:))
    stopflag=1;
    endindex=i;
    if beginindex<endindex

[temp,bestindex]=max(threshline(1,beginindex:endindex));
        bestindex=beginindex+bestindex-1;

thresh_threshline(1,beginindex:endindex)=thresh_threshline(1,beginindex
:endindex)*0;
            thresh_threshline(1,bestindex)=1;
        end
    end
end
if i<=length(thresh_threshline(1,:))
    endindex=i-1;
    if beginindex<endindex

[temp,bestindex]=max(threshline(1,beginindex:endindex));
        bestindex=beginindex+bestindex-1;

thresh_threshline(1,beginindex:endindex)=thresh_threshline(1,beginindex
:endindex)*0;
            thresh_threshline(1,bestindex)=1;
        end
    end
end

end

end

threshlineindex=find(thresh_threshline==1);
if s==1
    newsidata=nspecsmoothed_mat_temp(:,firstindex);
    peakmat=thresh_threshline;
else
    peakmat=[peakmat;thresh_threshline];
    newsidata=[newsidata
nspecsmoothed_mat_temp(:,firstindex)];
end
num_peaks_all=length(threshlineindex(1,:));

if seeplots==1
    %plot(nspecsmoothed_mat_temp(:,firstindex));
    for j=1:1:num_peaks_all

line([threshlineindex(1,j);threshlineindex(1,j)],[1;0]);
        end

end

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% End of peak filtering

```

```

%%%%%%%%%neric; modified to reduce lines of code RWC; Find the
peak intensities by baselines at peaks found with SIM

```

```

peak_max=zeros(length(threshlineindex(1,:)),1);

```

```

for p=1:1:num_peaks_all
    peak_max(p,1)=sidata(threshlineindex(1,p),1); %finds
the y value for each pixel in threshlineindex
end

```

```

sdat=nspecsmoothed_mat_temp(:,firstindex);
if seeplots==1
    plot(sdat);
end
threshlineindex=find(peakmat(s,:)==1);
num_peaks_all=length(threshlineindex(1,:));
if threshlineindex(1,1)==1 % this block avoids the first
spectrum pixel from being a peak position

```

```

threshlineindex=threshlineindex(1,2:length(threshlineindex(1,:)));
num_peaks_all=length(threshlineindex(1,:));
end
if
threshlineindex(1,length(threshlineindex(1,:)))==length(sdat(:,1)) %
this block avoids the last spectrum pixel from being a peak position

```

```

threshlineindex=threshlineindex(1,1:length(threshlineindex(1,:))-1);
num_peaks_all=length(threshlineindex(1,:));
end

```

```

%-----Peak heights to the baseline-----

```

```

real_peak_hts=zeros(size(threshlineindex));

```

```

if exist('num_peaks_all')==1

```

```

    keptpeaksindex=0;

```

```

    keptpeakhts=0;

```

```

    for i=1:1:num_peaks_all

```

```

        if num_peaks_all==[1 1]|(i==1&num_peaks_all>1)

```

```

            % if there is only one peaks

```

```

            lefty=[sdat(1:threshlineindex(1,i)-1,1)];

```

```

            ldeltx=[1:threshlineindex(1,i)-1]';

```

```

            ldeltx=flipud(ldeltx);

```

```

            ldely=sdat(threshlineindex(1,i),1)-lefty;

```

```

            if num_peaks_all==[1 1]

```

```

righty=[sdat(threshlineindex(1,i)+1:length(sdat(:,1)),1)];

```

```

            rdeltx=[1:(length(sdat(:,1)))-

```

```

threshlineindex(1,i)]';

```

```

            rdely=righty-sdat(threshlineindex(1,i),1);

```

```

            elseif i==1&num_peaks_all>1 %for first peak

```

```

righty=[sdat(threshlineindex(1,i)+1:threshlineindex(1,i+1)-1,1)];

```

```

rdeltx=[1:(threshlineindex(1,i+1)-1)-
threshlineindex(1,i)]';
rdelty=righty-sdat(threshlineindex(1,i),1);
end
elseif i==num_peaks_all&num_peaks_all>1|
(i>1&i<num_peaks_all) %for last peak and middle
lefty=[sdat(threshlineindex(1,i-
1)+1:threshlineindex(1,i)-1,1)];
ldeltx=[1:threshlineindex(1,i)-
threshlineindex(1,i-1)-1]';
ldeltx=flipud(ldeltx);
ldelty=sdat(threshlineindex(1,i),1)-lefty;
if i==num_peaks_all&num_peaks_all>1

righty=[sdat(threshlineindex(1,i)+1:length(sdat(:,1)),1)];
rdeltx=[1:(length(sdat(:,1)))-
threshlineindex(1,i)]';
rdelty=righty-sdat(threshlineindex(1,1),1);
elseif i>1&i<num_peaks_all % for all middle
peaks

righty=[sdat(threshlineindex(1,i)+1:threshlineindex(1,i+1)-1,1)];
rdeltx=[1:(threshlineindex(1,i+1)-1)-
threshlineindex(1,i)]';
rdelty=righty-sdat(threshlineindex(1,i),1);
end
end
end
lslope=ldelty./ldeltx;
[lslopemax,lslopemaxindex]=max(lslope(:,1));
rslope=rdelty./rdeltx;
[rslopemax,rslopemaxindex]=min(rslope(:,1));
if num_peaks_all==[1 1]|i==1&num_peaks_all>1
x1=lslopemaxindex;
x2=threshlineindex(1,i)+rslopemaxindex;
y1=sdat(lslopemaxindex,1);
y2=sdat(threshlineindex(1,i)+rslopemaxindex,1);
elseif
i>1&i<num_peaks_all|(i==num_peaks_all&num_peaks_all>1) %for last peak%
for all middle peaks
x1=threshlineindex(1,i-1)+lslopemaxindex;
x2=threshlineindex(1,i)+rslopemaxindex;
y1=sdat(threshlineindex(1,i-
1)+lslopemaxindex,1);
y2=sdat(threshlineindex(1,i)+rslopemaxindex,1);
end

%%%The above part of the loop works, now we need
to walk the line down using slopes%%%%%%%%%%%%%%
lefty_new=lefty;
ldeltx_new=x2-threshlineindex(1,i)+ldeltx;
ldelty_new=y2-lefty_new;
lslope_new=ldelty_new./ldeltx_new;

[lslopemax_new,lslopemaxindex_new]=max(lslope_new(:,1));
righty_new=righty;
rdeltx_new=threshlineindex(1,i)-x1+rdeltx;
rdelty_new=righty_new-y1;

```

```

rslope_new=rdelty_new./rdeltx_new;

[rslopemax_new,rslopemaxindex_new]=min(rslope_new(:,1));
if num_peaks_all==[1 1]|(i==1&num_peaks_all>1)
    x1new=lslopemaxindex_new;
    x2new=threshlineindex(1,i)+rslopemaxindex_new;
    y1new=sdat(lslopemaxindex_new,1);

y2new=sdat(threshlineindex(1,i)+rslopemaxindex_new,1);
elseif
i>1&i<num_peaks_all|(i==num_peaks_all&num_peaks_all>1) %for last peak%
for all middle peaks
    x1new=threshlineindex(1,i-
1)+lslopemaxindex_new;
    x2new=threshlineindex(1,i)+rslopemaxindex_new;
    y1new=sdat(threshlineindex(1,i-
1)+lslopemaxindex_new,1);

y2new=sdat(threshlineindex(1,i)+rslopemaxindex_new,1);
end

while [x1,y1,x2,y2]~=[x1new,y1new,x2new,y2new];
    x1=x1new;
    y1=y1new;
    x2=x2new;
    y2=y2new;
    lefty_new=lefty;
    ldeltx_new=x2-threshlineindex(1,i)+ldeltx;
    ldelty_new=y1-lefty_new;
    lslope_new=ldelty_new./ldeltx_new;

[lslopemax_new,lslopemaxindex_new]=max(lslope_new(:,1));
    righty_new=righty;
    rdeltx_new=threshlineindex(1,i)-x1+rdeltx;
    rdelty_new=righty_new-y2;
    rslope_new=rdelty_new./rdeltx_new;

[rslopemax_new,rslopemaxindex_new]=min(rslope_new(:,1));

if num_peaks_all==[1 1]|(i==1&num_peaks_all>1)
    x1new=lslopemaxindex_new;

x2new=threshlineindex(1,i)+rslopemaxindex_new;
    y1new=sdat(lslopemaxindex_new,1);

y2new=sdat(threshlineindex(1,i)+rslopemaxindex_new,1);
elseif
i>1&i<num_peaks_all|(i==num_peaks_all&num_peaks_all>1) %for last peak%
for all middle peaks
    x1new=threshlineindex(1,i-
1)+lslopemaxindex_new;

x2new=threshlineindex(1,i)+rslopemaxindex_new;
    y1new=sdat(threshlineindex(1,i-
1)+lslopemaxindex_new,1);

```



```

y2new=sdat(threshlineindex(1,i)+rslopemaxindex_new,1);
    end

    end
    if seeplots==1
        h=line([x1new,x2new],[y1new,y2new]);
        set(h,'color',[1 0 0],'linewidth',[1.4]);
    end
    %%%The following code is used to draw a line from
the peak center to the baseline%%%%%%%%%%5
    a=abs(x2new-x1new);
    b=abs(y2new-y1new);
    c=abs(sqrt(a^2+b^2));
    bt=abs(acos(a/c)); %bt stands for "b theta". after
conversion, bt is now in degrees. I'm not sure if this is adequate
since 57.2957 is approx.
    xline=threshlineindex(1,i);
    at=abs(2*4*atan(1)-(1.5705+bt)); %at stands for "a
theta". it's result is in degrees
    new_a=abs(x2new-xline);
    new_b=abs((new_a/sin(at))*sin(bt));
    if y2new<y1new
        y2new=y2new+new_b;
        if seeplots==1

peak_ht_real=line([xline,xline],[y2new,sdat(threshlineindex(1,i),1)]);
        end
    else
        y2new=y2new-new_b;
        if seeplots==1

peak_ht_real=line([xline,xline],[y2new,sdat(threshlineindex(1,i),1)]);
        end
    end
    if seeplots==1
        set(peak_ht_real,'color',[1 0
0],'linewidth',[1.4]);
    end
    real_peak_hts(1,i)=sdat(threshlineindex(1,i),1)-
y2new; %Gives peak heights

    if real_peak_hts(1,i)>=4*noise
        keptpeaksindex=[keptpeaksindex
threshlineindex(1,i)];
        keptpeakhts=[keptpeakhts
sdat(threshlineindex(1,i),1)-y2new];
    end

    end%%end of i loop
end %%end of if exist num_peaks_all
%

keptpeaksindex=keptpeaksindex(2:length(keptpeaksindex(1,:)));
keptpeakhts=keptpeakhts(2:length(keptpeakhts(1,:)));
num_keptpeaks_all=length(keptpeaksindex(1,:));

```

```

        if seeplots==1
            finalfig=figure;
            plot(nspecssmoothed_mat_temp(:,firstindex));
            title('Final Figure');
            for j=1:1:num_keptpeaks_all

line([keptpeaksindex(1,j);keptpeaksindex(1,j)], [1;0]);
            end

        end

        if seeplots==1
            %plot(spec(:,s));
            end
            %lorplots=menu('Give all lorentzian replacements uniform
intensity?', 'No', 'Yes'); %works regardless in findpeaks24
            lorplots=2;
            lor_length=length(spec(:,1)); %5*fwhm;
            vect_lor = zeros(num_peaks_all,lor_length);
            for j=1:1:num_keptpeaks_all
                for n=1:1:lor_length
                    if lorplots==1
                        %vect_lor(j,n) = keptpeakhts(1,j)/(fwhm.^2 +
(n-keptpeaksindex(1,j))^2); % keptpeakhts(1,j)*(fwhm) on top
                        vect_lor(j,n) = (keptpeakhts(1,j))/(1+((n-
keptpeaksindex(1,j))/(fwhm/3))^2);
                    elseif lorplots==2
                        vect_lor(j,n) = (keptpeakhts(1,j))/(1+((n-
keptpeaksindex(1,j))/(fwhm/3))^2);
                    end
                end
            end
            end
            if length(vect_lor(:,1))==1
                vect_lormat(:,s)=vect_lor';
            else
                vect_lormat(:,s)=sum(vect_lor)';
            end

            %if normal==1
            minvect_lormat=min(vect_lormat(:,s));
            maxvect_lormat=max(vect_lormat(:,s));
            rangevect_lormat= maxvect_lormat-minvect_lormat;
            vect_lormat(:,s)=(vect_lormat(:,s)-
minvect_lormat)./rangevect_lormat;
            %end

            if seeplots==1 %Smooth and Lorentzian replaced

                for j=1:1:num_keptpeaks_all

line([caldata_xmat(keptpeaksindex(1,j),s);caldata_xmat(keptpeaksindex(1
,j),s)], [max(nspecssmoothed_mat_temp(:,firstindex));min(nspecssmoothed_ma
t_temp(:,firstindex))]);
                end
            end
        end
    end
end

```

```

%end %s loop

%%%%%%%%%neric end
if seeplots==1
    %plot(vect_lormat);
end

offset=.6;
stack_lormat=vect_lormat.*0;
for j=1:1:length(vect_lormat(1,:))
    stack_lormat(:,j)=vect_lormat(:,j)+offset*(j);
end

if seeplots==1
    %plot(caldata_xmat,stack_lormat); %Lorentzian replaced
daily pen spectra and penref
    axis([min(caldata_xmat(:,1)) max(caldata_xmat(:,1)) 0
max(max(stack_lormat))+offset]);
    title('Lorentzian Band Replacement Spectra');
    xlabel('Raman Shift');
    ylabel('Normalized Intensity');
    %pause
end

%Calibration section
if s==1
    daily_pen_cal_mat=flipud(sortrows([keptpeakhts'
keptpeaksindex'],1));
else

    penref_cal_mat=flipud(sortrows([keptpeakhts'
keptpeaksindex'],1));

    ClosestMatchSpectra2; %Makes sure the top 5 peaks in
the penref corresponds to the daily pen cal mat

    avgpeak_shift=round((sum(daily_pen_cal_mat_new(1:5,2)-
penref_cal_mat(1:5,2)))/5);
    %positive values for avgpeak_shift indictes that the
indices of the penref spectrum should be increased by the
avgpeak_shift. For negative avgpeak_shift, the penref indices should
be decreased by the avgpeak_shift.
    refpeakmatnew=[refpeakmat(:,1)+ avgpeak_shift,
refpeakmat(:,2)];

    %OR we could have plotted the pixels for the penref
versus the change in value at the keptindex position, then polyfit;

%%This is a third order calibration section; A first order calibration
follows
    polyfitorder=3;

[p,sss]=polyfit(refpeakmatnew(:,1),refpeakmatnew(:,2),polyfitorder);
%Two separate polyfits using preselected order, pixel & wavelength

```

```

        waves_fromrefpeakmatnew=p(1,1)*refpeakmatnew(:,1).^3 +
p(1,2)*refpeakmatnew(:,1).^2 + p(1,3)*refpeakmatnew(:,1)+ p(1,4);

        euclid_dist=(sum((refpeakmatnew(:,2)-
waves_fromrefpeakmatnew).^2 ))^.5 %waves_fromrefpeakmatnew are shifted

        if euclid_dist>1 %if euclidean distance is sufficiently
small
            saveflag=0;
        end

        pixels=[1:1340];
        waves_frompix=p(1,1)*pixels.^3 + p(1,2)*pixels.^2 +
p(1,3)*pixels + p(1,4);

        if seeplots==1

%plot(refpeakmatnew(:,1),refpeakmatnew(:,2),pixels,waves_frompix);
        %pause;
        end

        wavenums=1./(waves_frompix*10^(-7));
        deltawavenums=laserwavenum-wavenums;
        %Background subtraction and application of the shift
the subtracted data
        caldata=[deltawavenums' sidata(:,2)-sidata(:,3)];
%Calibrate the penfirst then run the same routine against the data?

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%The section below is for a first order fit
        polyfitorder1=1;

[p,sss]=polyfit(refpeakmatnew(:,1),refpeakmatnew(:,2),polyfitorder1);
%Two separate polyfits using preselected order, pixel & wavelength

        waves_fromrefpeakmatnewfo=p(1,1)*refpeakmatnew(:,1)+
p(1,2);

        euclid_distfo=(sum((refpeakmatnew(:,2)-
waves_fromrefpeakmatnewfo).^2 ))^.5 %waves_fromrefpeakmatnew are
shifted

        if euclid_distfo>1 %if euclidean distance is
sufficiently small
            saveflag=0;
        end

        pixels=[1:1340];
        waves_frompixfo=p(1,1)*pixels + p(1,2);

        if seeplots==1

```

```

plot(refpeakmatnew(:,1),refpeakmatnew(:,2),'r*',pixels,waves_frompixfo)
;
        %pause;
        end

        wavenums=1./(waves_frompix*10^(-7));
        deltawavenums=laserwavenum-wavenums;

        %Create matrix with the x and y data to be append to a .csv file

        %y = caldata(:,2)';
        %x1=[1,3,3,4];
        %x2=x1';
        %fid =
fopen('C:\Users\Antoinette\Desktop\RC\Gradwork\spectradata.txt','a');

%csvwrite('c:\Users\Antoinette\Desktop\RC\Gradwork\spectradata.txt',
y); %Here is the data written as csv, can make it go int variable?

        %fclose(fid);

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

        %Create sdata.csv for php upload
        %Note that data will be space delimited for excel
insertion
        %of .txt files
        % For clarity create a text list for the sample number
then
        % a csv for the data. Next append the sample list to
the csv
        % for upload

        %iniate i for the cookid
        i=5;
        while(rawspemat(dline,i)~='_')
            i=i+1;
        end

        j=i-1;

        cookid=(rawspemat(dline,1:j))

        fid =
fopen('c:\Users\Antoinette\Desktop\RC\Gradwork\sdata5.txt', 'a');
%Location of the shift corrected plots for the samples

```

```

        fprintf(fid, '');
        fprintf(fid, cookid);
        fprintf(fid, '');
        fprintf(fid, ', ');

        fprintf(fid, '');
        fclose(fid);
        fid
=fopen('c:\Users\Antoinette\Desktop\RC\Gradwork\sdata5.txt', 'a');
%good

        dlmwrite
('c:\Users\Antoinette\Desktop\RC\Gradwork\sdata5.txt', y, '-append');
        fprintf(fid, '');
        fprintf(fid, ', ');

        fclose(fid); %good

        %Tracking number
        fid
=fopen('c:\Users\Antoinette\Desktop\RC\Gradwork\sdata5.txt', 'a');
%good

        fprintf(fid, '');
        dlmwrite
('c:\Users\Antoinette\Desktop\RC\Gradwork\sdata5.txt', dline, '-
append');
        %fid =
fopen('c:\Users\Antoinette\Desktop\RC\Gradwork\sdata4.txt', 'a');
        fprintf(fid, ""\n"); %good

        fclose(fid); %good

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% This section makes print out of the spectra image
% name association for php. Optional

i=1;

```

```

while (rawspemat (dline,i) ~='_')
    i=i+1;
end

j=i-1;

cookid=(rawspemat (dline,1:j));

title(cookid); %Need a variable for the mineral name or
use php/sql
xlabel('Wavenumber (cm -1)');
ylabel('Intensity');
%Check axis maximum, it won't plot if all zeroes or max
is
%negative
plotmax=max(sidata(:,2)-sidata(:,3));
axis([0 max(deltawavenums') 0 max(sidata(:,2)-
sidata(:,3))]);
set(gca,'LineWidth', 2)

fl='C:\Users\Antoinette\Desktop\RC\Gradwork\Spectra\';
ft='.jpg';
finalfile=[fl cookid ft];
%saveas(h,finalfile,'jpg')
imagefileext=[cookid ft ',''];
fid =
fopen('c:\Users\Antoinette\Desktop\RC\Gradwork\raman_mindb\imagefileext
.txt', 'a'); %Location of the shift corrected plots for the samples
%rite=[cookid '\n'];

fprintf(fid, imagefileext); %Return Graph

fclose(fid)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

%Creates id.txt for php

newcookid{z}=[cookid];
z=z+1;
%end
ccookid=[cookid ',''];

fid =
fopen('c:\Users\Antoinette\Desktop\RC\Gradwork\raman_mindb\graphid.txt'
, 'a'); %Location of the shift corrected plots for the samples
rite=[cookid '\n'];

fprintf(fid, ccookid); %Return graph

fclose(fid);

```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```

```
        if seeplots==1
            resultfig=figure;

            end
            shiftlog=[shiftlog; dline avgpeak_shift];

            if seeplots==1

%plot(refpeakmatnew(:,1),refpeakmat(:,2),refpeakmat(:,1),refpeakmat(:,2
));
                %pause
            end

                close all

                    end
                end
            end
            if saveflag==1
                %save file
            end
        end

fclose('all');
```



## APPENDIX I:

### SIM Matlab file sorting program rf10\_20\_092

```
% Original written by Jon Damsel and John F.Turner II; modified by
Robert Cannon for automation

% Be sure the directory and file naming conventions are adhered to:
%
% Directories follow this convention:
% MM_DD_YY(q)
% Data Files follow this convention:
% A####(q)_####nm_####dcm_(#,##,###,...)(.#,
.##)s_2(bg).(spe,SPE) where () are wildcards
% Penlamp Files follow this convention:
% (neon, krypton)pen__####nm_####dcm.(spe,SPE) where () are
wildcards
%
% Each Directory should have not more than 1 penlamp spectra. If
two or more exist, they should be placed in new directories along with
the corresponding raw and bg files.
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

close all;
%clear;
clc;

% find directory contents of c:\c1\damsel\mindb
%[filename path]=uigetfile('*..*','Please Open Directory for
Calibration');
%thepath=path(1:length(path(1,:))-1);
%path='c:\c1\damsel\mindb;
%path='G:\Backup 11-28-11\Gradwork\mindb2alldata'; %This from the jump
drive
path='C:\Users\Antoinette\Desktop\RC\Gradwork\mindb2alldata'; %This
from the jump drive
mindbdir=dir(path);

%determine which directories inside of c:\c1\damsel\mindbwe wish to
calibrate
gooddir=0;
file=0;
baddir=0;
for j=1:length(mindbdir(:,1))
    if mindbdir(j,1).isdir==1
        dirname=mindbdir(j,1).name;
        if length(dirname(1,:))==8|length(dirname(1,:))==9
            if dirname(1,1)=='0'|dirname(1,1)=='1'
                if
dirname(1,2)=='0'|dirname(1,2)=='1'|dirname(1,2)=='2'|dirname(1,2)=='3'
|dirname(1,2)=='4'|dirname(1,2)=='5'|dirname(1,2)=='6'|dirname(1,2)=='7'
|dirname(1,2)=='8'|dirname(1,2)=='9'
```

```

        if dirname(1,3)=='_'
            if
dirname(1,4)=='0'|dirname(1,4)=='1'|dirname(1,4)=='2'|dirname(1,4)=='3'
                if
dirname(1,5)=='0'|dirname(1,5)=='1'|dirname(1,5)=='2'|dirname(1,5)=='3'
|dirname(1,5)=='4'|dirname(1,5)=='5'|dirname(1,5)=='6'|dirname(1,5)=='7'
'|dirname(1,5)=='8'|dirname(1,5)=='9'
                    if dirname(1,6)=='_'
                        if
dirname(1,7)=='0'|dirname(1,7)=='1'|dirname(1,7)=='2'|dirname(1,7)=='3'
|dirname(1,7)=='4'|dirname(1,7)=='5'|dirname(1,7)=='6'|dirname(1,7)=='7'
'|dirname(1,7)=='8'|dirname(1,7)=='9'
                            if
dirname(1,8)=='0'|dirname(1,8)=='1'|dirname(1,8)=='2'|dirname(1,8)=='3'
|dirname(1,8)=='4'|dirname(1,8)=='5'|dirname(1,8)=='6'|dirname(1,8)=='7'
'|dirname(1,8)=='8'|dirname(1,8)=='9'
                                if length(dirname(1,:))==8
                                    gooddir=[gooddir j];
                                end

                                if length(dirname(1,:))==9
                                    letters=['a' 'b' 'c' 'd' 'e' 'f'
'g' 'h' 'i' 'j' 'k' 'l' 'm' 'n' 'o' 'p' 'q' 'r' 's' 't' 'u' 'v' 'w' 'x'
'y' 'z' 'A' 'B' 'C' 'D' 'E' 'F' 'G' 'H' 'I' 'J' 'K' 'L' 'M' 'N' 'O' 'P'
'Q' 'R' 'S' 'T' 'U' 'V' 'W' 'X' 'Y' 'Z'];
                                    for i=1:1:length(letters(1,:))

                                        if
sum(find(dirname(1,9)==letters(1,i)))
                                            %keep this directory
                                            gooddir=[gooddir j];
                                        end
                                    end
                                end
                            else
                                baddir=[baddir j];
                            end
                        else
                            baddir=[baddir j];
                        end
                    else
                        baddir=[baddir j];
                    end
                else
                    baddir=[baddir j];
                end
            else
                baddir=[baddir j];
            end
        else
            baddir=[baddir j];
        end
    end
end

```

```
        end
    else
        baddir=[baddir j];
    end
else
    baddir=[baddir j];
end
else
    file=[file j];
end
end
gooddir=gooddir(2:length(gooddir(1,:)));
baddir=baddir(2:length(baddir(1,:)));
gooddir_strmat=strvcat(mindbdir(gooddir(1,:)).name);
baddir_strmat=strvcat(mindbdir(baddir(1,:)).name);
```

## APPENDIX J:

### SIM initiation program pb\_next

%Original written by Jon Damsel and John F. Turner II; modified by  
Robert W. Cannon for automation

```
%close(frame1_fig);
q=0;
spemat='.spe';
dirmat='dir';
rawspemat='2.spe';
exactraw='exactraw';
bgspemat='2bg.spe';
exactbgspemat='exactbg';
penspemat='pen.spe';
dspemath='d';
otherspemat='other';
dospemat='do';
otherexactrawl='oerl';
allrawspemat='allraw';
allraw='allraw';

for d=1:1:length(gooddir(1,:))
    pathname=[path '\\' mindbdir(gooddir(1,d),1).name];
    subdir1=dir(pathname);
    penflag=0;
    for s=1:1:length(subdir1(:,1))
        tempstr=subdir1(s,1).name;
        if
length(tempstr(1,:))>8&(~isempty(findstr(tempstr(1,:),'.SPE')))
            if strcmp(tempstr(1,length(tempstr(1,:))-
3:length(tempstr(1,:))),'.SPE')
                spemat=strvcat(spemat,subdir1(s,1).name);%1
                dirmat=strvcat(dirmat,[pathname '\\']);
                if
(~isempty(findstr('2.SPE',tempstr)))&isempty(findstr(tempstr,'pen'))
                    genbgname=[tempstr(1,1:length(tempstr(1,:))-4)
'bg.SPE'];
                    mnametemp='tmp';
                    for m=1:1:length(subdir1(:,1))
                        mnametemp=strvcat(mnametemp,subdir1(m,:).name);
                        if ~isempty(findstr(subdir1(m,:).name,'pen'))
                            exactpenmat=subdir1(m,:).name;
                            penflag=1;
                        end
                    end
                    bgindex=strmatch(genbgname,mnametemp,'exact');
                    if ~isempty(bgindex)
                        if length(bgindex(:,1))==1
                            if penflag==1
                                nmpos=findstr(exactpenmat,'nm');%4
                                exactpenlaser=exactpenmat(1,nmpos-3:nmpos-1);
```

```

        rawnmpos=findstr(tempstr,'nm');
        rawlaser=tempstr(1,rawnmpos-3:rawnmpos-1);
        if
~isempty(rawlaser)&~isempty(exactpenlaser)&rawlaser==exactpenlaser
            rawspemat=strvcat(rawspemat,tempstr);%5
            exactraw=tempstr;
            bgspemat=strvcat(bgspemat,genbgname);

exactbgspemat=strvcat(exactbgspemat,genbgname);
            exactbg=genbgname;
            penspemat=strvcat(penspemat,exactpenmat);
            dspemath=strvcat(dspemath,[pathname '\\']);
            else otherspemat=strvcat(otherspemat,tempstr);
                dospemat=strvcat(dospemat,[pathname '\\']);
            end
            else otherspemat=strvcat(otherspemat,tempstr);
                dospemat=strvcat(dospemat,[pathname '\\']);
            end
        end
        end
        else
            otherexactrawl=tempstr;
        end
    elseif ~(isempty(findstr(tempstr,'2bg.SPE')))
        if strcmp(tempstr(1,6:8),'all')
            q=q+1;
            allbgname=tempstr;
            catname=tempstr(1,1:5);
            endname=tempstr(1,length(tempstr(1,:))-
3:length(tempstr(1,:)));
            for t=1:1:length(subdir1(:,1))
                ttempstr=subdir1(t,:).name;
                if ~isempty(findstr(subdir1(t,:).name,'pen'))
                    penmat=subdir1(t,:).name;
                    penendname=ttempstr(1,length(ttempstr(1,:))-
3:length(ttempstr(1,:)));
                    penflag=1;
                    nmpos=findstr(penmat,'nm');%4
                    penlaser=penmat(1,nmpos-3:nmpos-1);
                    if strcmp(endname,penendname,4)
                        penname=penmat;
                        for w=1:1:length(subdir1(:,1))
                            if
length(subdir1(w,:).name)>8&(~isempty(findstr(subdir1(w,:).name,'2.SPE'
)))
                                if
~isempty(findstr(catname,subdir1(w,:).name))&penflag==1
                                    allrawname=(subdir1(w,:).name);
                                    bgnmpos=findstr(allbgname,'nm');
                                    bglaser=allbgname(1,bgnmpos-
3:bgnmpos-1);
                                    if bglaser==penlaser
                                        rawspemat=strvcat(rawspemat,allrawname);

                                        allrawspemat=strvcat(allrawspemat,allrawname);
                                        allraw=allrawname;

```

```

bgspemat=strvcat (bgspemat, allbgname);

penspemat=strvcat (penspemat, penname);

dspemath=strvcat (dspemath, [pathname '\\']);
    end
    end
    end
    end
    end
    end
    end
    elseif (strncmp (tempstr, exactbg, length (exactbg)))==0
        otherspemat=strvcat (otherspemat, tempstr);
        dospemat=strvcat (dospemat, [pathname '\\']);
    end
    elseif isempty (findstr (tempstr, 'pen'))
        otherspemat=strvcat (otherspemat, tempstr);
        dospemat=strvcat (dospemat, [pathname '\\']);
    end
    if
strncmp (otherexactraw1, tempstr, length (tempstr)) ==1 & strcmp (allraw, tempstr, 5) ==0
        otherspemat=strvcat (otherspemat, tempstr);
        dospemat=strvcat (dospemat, [pathname '\\']);
    end
    end
    end
    clear bgindex
    end
end

%mindbdir (gooddir (1, d), 1).name %debugger
%%Now Calibrate Spectra in the dth directory
rawspemat=rawspemat (2:length (rawspemat (:, 1)), :);
bgspemat=bgspemat (2:length (bgspemat (:, 1)), :);
penspemat=penspemat (2:length (penspemat (:, 1)), :);
spemat=spemat (2:length (spemat (:, 1)), :);
dirmat=dirmat (2:length (dirmat (:, 1)), :);
dspemath=dspemath (2:length (dspemath (:, 1)), :);
otherspemat=otherspemat (2:length (otherspemat (:, 1)), :);
dospemat=dospemat (2:length (dospemat (:, 1)), :);
fprintf ('Calibrating %d %s\n', d, mindbdir (gooddir (1, d), 1).name);

a='DONE'

```

## APPENDIX K:

### SIM Matlab peak matching ClosestMatchSpectra2

```
%Robert W. Cannon

%Finds the difference and index from the subtraction of one peak matrix
to another for each element in the first; used to keep the correct peak
order

penref_cal_positions=penref_cal_mat(1:5,2);

j=0;

for j=1:length(penref_cal_positions)
    [c,i] = min(abs(penref_cal_positions(j) - daily_pen_cal_mat(:,2)));
    et(j,:)= [c i];
end

daily_ref_diff=et(:,1); %Differences in the closest matches
daily_min_indexes=et(:,2); %Indexes of the closest matches in second
matrix

%Returns numbers the most closely match in matrix 2 to the known values
%in matrix 1

for h=1:length(daily_min_indexes)

daily_pen_cal_mat_new(h,:)=daily_pen_cal_mat(daily_min_indexes(h),:);
%most intense
end
```

## APPENDIX L:

### Ramindex main page HTML "test28.html"

```
<?xml version="1.0" encoding="utf-8"?>
<!DOCTYPE html PUBLIC "-//W3C//DTD XHTML 1.0 Transitional//EN"
"http://www.w3.org/TR/xhtml1/DTD/xhtml1-transitional.dtd">
<html xmlns="http://www.w3.org/1999/xhtml">

<meta
http-equiv="content-type" content="text/html;
charset=encoding" />

<title> RamIndex - a standardized spectral database</title>

<!--Library Scripts and CSS-->

<link rel="icon" href="/html/images/RamIndexIcon.ico" type="image/x-
icon"/>
<link rel="shortcut icon" href="/html/images/RamIndexIcon.ico"
type="image/x-icon"/>

<!--link rel="stylesheet" href="C:/xampp/htdocs/html/tab.css"
type="text/css" />-->

<link rel="stylesheet" type="text/css"
href="/html/jquery/jqueryui/css/ui-lightness/jquery-ui-
1.8.16.custom2.css"/>

<!--Javascript Library Files -->
<script src="/html/jquery-1.7.1.js"></script>
<script src="/html/jquery/js/jquery-ui-1.8.16.custom.min.js"></script>
<script src="/html/spin.min.js"></script>

<script>

        $(function() {

            function split( val ) {
                return val.split( /\s*/ );
            }
            function extractLast( term ) {
                return split( term ).pop();
            }

            $( "#tags" )
            // don't navigate away from the field on tab when selecting an item
                .bind( "keydown" )

            .autocomplete({
                source: function( request, response ) {
                    $.getJSON( "/html/fetchCriteria2.php", {
                        term: extractLast( request.term )
                    }, response );
                },
                search: function() {
                    // custom minLength
                    var term = extractLast( this.value );
                    if ( term.length < 2 ) {
```



```

        return false;
    }
},
focus: function() {
    // prevent value inserted on focus
    return false;
},
select: function( event, ui ) {
    var terms = split( this.value );
    // remove the current input
    terms.pop();
    // add the selected item
    terms.push( ui.item.value );
    // add placeholder to get the comma-and-
space at the end
    terms.push( " " );

    this.value = terms.join(",");
    return false;
}
}
});
});
</script>
<script type="text/javascript">
    $(document).ready(function() {
//Filter Button icon
$(".sb").button({
icons: {primary: 'ui-icon-triangle-1-s' }
});

//Ajax activity indicator
var opts = {
    lines: 7, // The number of lines to draw
    length: 7, // The length of each line
    width: 4, // The line thickness
    radius: 10, // The radius of the inner circle
    rotate: 0, // The rotation offset
    color: '#000', // #rgb or #rrggbb
    speed: 1, // Rounds per second
    trail: 60, // Afterglow percentage
    shadow: false, // Whether to render a shadow
    hwaccel: false, // Whether to use hardware acceleration
    className: 'spinner', // The CSS class to assign to the spinner
    zIndex: 2e9, // The z-index (defaults to 2000000000)
    top: 72, // Top position relative to parent in px
    left: 82 // Left position relative to parent in px
};

var optsa = {
    lines: 7, // The number of lines to draw

```

```

length: 7, // The length of each line
width: 4, // The line thickness
radius: 10, // The radius of the inner circle
rotate: 0, // The rotation offset
color: '#000', // #rgb or #rrggbb
speed: 1, // Rounds per second
trail: 60, // Afterglow percentage
shadow: false, // Whether to render a shadow
hwaccel: false, // Whether to use hardware acceleration
className: 'spinnera', // The CSS class to assign to the spinner
zIndex: 2e9, // The z-index (defaults to 2000000000)
top: 72, // Top position relative to parent in px
left: 82 // Left position relative to parent in px
};

var target = document.getElementById('activit');
var spinner = new Spinner(opts).spin(target);

var targeta = document.getElementById('activita');
var spinnera = new Spinner(optsa).spin(targeta);

//Clears the filters
$('#dd').val("Any");

var select = jQuery('.fdd');

select.val(jQuery('options:first', select).val());

//Hides activity splash
//$(document).ajaxStop(function(){
//$('#activit').hide()
//});

//Show activity via button
$('#tagsb').click(function(){
$('#content').empty();
$('#activit').show().ajaxStop(function(){
$('#activit').hide();
});
});

});

$(".beta").hover(
function(){
//var value2 = $(this).text();
var let= $(this).attr('value');
//$("#alp").text(value2);
$("#alp").text(let);
});
});

$(document).ready(function(){

//Return to the splash screen if the logo is clicked;
$('#logo').click(function(){

```

```

//alert("go to home");
window.location = '/';

});

//Return to the splash screen with the home link

$('#home').click(function(){

//alert("go to home");
window.location = '/';

});

//Load results into the leftBar

function aLoad() {

if(request){
request.abort();
}

var request=
$('#leftBar').load('/html/ramindex_displaydb31.php',{mineralname:
$('#tags').val(),filters:data });
$('#gph').empty();

return false;
}

var data="Ma";
$('#tagsb').click(aLoad);

});

</script>

<!--Heads up display-->

<script>

$(function(){

$("#tags").focusout(function () {
var value = $(this).val();
//var comma = ",";
//alert(comma);
//alert($(this).val()+comma);
//apv=$(this).val()+comma);

//$("#tags").val(apv);

//$("#mn").text(value+comma+" ");
$("#mn").text(value);

}).keyup();

```

```

    });
</script>

<script>

$(document).ready(function(){

    $('#reload').click(function(){

window.location.reload();

    });
    });

    //For the dropdown list (dl)
    $(document).click(function(){
    $('#dl').mouseleave(function(){
    $('#dl').hide();

    });
    });

//For the tags box to add a comma on focus mouseleave
$('#tags').mouseleave(function(){
//alert("mouse out add the comma");
});

</script>

<script><!--For alphabet character-->

$(function(){

    $(".beta").click(function () {

//$("#dl").hide();

    //var value2 = $(this).text();

    var let= $(this).attr('value');
    //$("#alp").text(value2);
    $("#alp").text(let);

        var let= $(this).attr('value');
        $('#dl').load('/html/cbox7.php', {aletter:let});

    //return false;

    var shift = $(this).attr("shift");
    $("#alp2").text(shift);

$("#dl").css("margin-left",shift+"px");

    });

```

```

$(".beta").hover(function() {
    $(this).css("background","red");
    $(".beta").mouseout(function() {
        $(".beta").css("background","none")
    });
});

});

</script>

<script>
$(document).ready(function() {
    $('#div.body').show();
    $('#smd').empty();
    $('#leftBar').append($('TR')).addClass("item");
    $('#p.dbutton1').hide();
    $('#p.data1').hide();
});
</script>

<script type=text/javascript>

    $('#.item').click(function() {
//alert("this is a test");
//});
</script>

<script>
    $(function() {
        $('#progressbar').progressbar({
            value: 25
        });
    });
</script>

<script>
(function(){
$.fn.autoProgressbar = function(settings,value) {
//implementation will go here
return this;
};
});
</script>

<!--Script for graph selection-->

<!--Script for Log In & registration buttons-->

<script>

```

```

$(document).ready(function(){

    $('#loginb').toggle(function () {
        $('#login').toggle();
        $('#loginb').text("Hide");
    }, function(){
        $('#login').toggle();
        $('#loginb').text("Log In");
    });

    $("#logins").click(function () {
var username = $('#loginu').attr('value');
var password = $('#loginp').attr('value');

        $('#leftBar').load('/html/registration.php',{username:$('#loginu').
val(), password:password});

    });

    $("#loginn").click(function () {
var username = $('#loginu').attr('value');
var password = $('#loginp').attr('value');

    });

});

</script>

<style>
body{
font-family: Calibri;
}
.beta{
cursor:pointer;
}
#chem3,#chem4{
//display:none;
}
#container{
//margin-right:1000px;
//margin-left:850px;
width:300px;
color:white;
background:grey;

```

```

float:right;
height:100%;
}

#header{

background-color:#728C72;
padding-top:25px;
padding-left:14px;
padding-bottom:5px;
padding-right:5px;
color:white;
//font-size:16;
overflow:auto;
//background-image:url('C:\xampp\htdocs\html\images\ramindex');
}

#logo{

cursor:pointer;

}

#header2{

background-color:gray;
padding-top:10px;
padding-left:10px;
padding-bottom:5px;

color:white;
//font-size:95%;
display:none;
}

#df {
border-style:solid;
background-color:white;
width:148px;
height:160px;
display:none;
color:black;
z-index:100;
position:absolute;
margin-left:5.7em;
margin-top:30px;
}

#dl {

display:none;
height:300px;
width:200px;
border-color:black;
border-style:solid;
margin-top:-3px;
z-index:10;
position:absolute;
background:white;
}

#dd{
color:black;

```

```

}

#holder{
width:100%;
background-color:white; //blue;
overflow:auto;
//height: fixed;
}

#leftBar {

float: left;
width: 15%; //180px;
height:600px;
background: #728C72; // #EBEBEB;
overflow:auto;
padding:8px;

}

#leftBar a {

color:#B4E9F0;

}

#content {
float:top;
width: auto; //972px;
padding:9px;
//clear:both;
//height:;
overflow:auto;
//position:relative;

background-color: white; //red; // #cdcde6;
}

#rightBar {
float:right;
width: 15%; //169px;
background: #EBEBEB;
height:600px;
padding:8px;

}

#footer {
clear:both;
background:#DDDDDD;
height:20px;
//overflow:auto;
}

#f2{

float:right;

```



```

}

#csulink{

text-decoration:none;
color:black;

}

#combin, #multip {

width:200px;
display:none;
}

#progressbar{

width:500px;

}

#ip{

display:none;
z-index:11;
position:absolute;
}

#filters{

//width:300px;
//height:110px;
float:right;
color:white;
//margin-top:-125px;
//margin-left:850px;
margin-right:50px;
//position:absolute;
}

#help{

float:right;
color:white;
position:absolute;
//margin-left:220px;
//margin-top:10px;

}

#activit{

z-order:120;
width:212px; //400px;
height:212px; //400px;
border-color:black;
border-style:solid;
background-color:grey;
opacity:0.5;
position:absolute;
margin-left:40%;
margin-top:-40px;
padding-left:20px;

```

```

padding-top:20px;
display:none;

}

#activita{

z-order:120;
width:212px; //400px;
height:212px; //400px;
border-color:black;
border-style:solid;
background-color:grey;
opacity:0.5;
position:absolute;
margin-left:40%;
margin-top:-40px;
padding-left:20px;
padding-top:20px;
display:none;

}

.sb{

height:22px;
width:24px;
margin-top:0px;
//margin-left:px;
position:absolute;
//padding-left:0px;

}

.ui-button-icon-primary{
diplay:block;
margin-left:-6px;
}

#fd1{
margin-left:45px;
width:120px;
}

#fd2{
margin-top:2px;
margin-left:14px;
width:120px;
}

#fd3{
margin-top:2px;
margin-left:4px;
width:120px;
}

#login{
//background-color:yellow;
display:none;
}

#loginr{

display:none; //For display the logged in username

```

```

}

#home {

float:right;
margin-top:-20px;
//display:none;
cursor:pointer;
}

</style>

<div id="header">

<div id="home">
HOME&nbsp;
</div>

<div id="title">
<span id="logo">



</span>

<fieldset id=filters >
<legend style="color:white;">Filters</legend>

Color:

<select class="fdd" id="fd1">
  <option value="Any">Any</option>
  <option value="Red">Red</option>
  <option value="Green">Green</option>
  <option value="Blue">Blue</option>
  <option value="Yellow">Yellow</option>
  <option value="Opal">Opal</option>
  <option value="Black">Black</option>
  <option value="Brown">Brown</option>
  <option value="Gold">Gold</option>
</select> <br />
Chemistry:
<select class="fdd" id="fd2">
  <option value="Any">Any</option>
  <option value="carbonate">Carbonate</option>
  <option value="sulfate">Sulfate</option>
  <option value="nitrate">Nitrate</option>
  <option value="phosphate">Phosphate</option>
  <option value="oxide">Oxide</option>
  <option value="silicate">Silicate</option>
  <option value="silicate">Silicate</option>
<optgroup label=Elements>
<option value="hydrogren">1-Hydrogen</option>
<option value="helium">2-Helium</option>
<option value="lithium">3-Lithium</option>
<option value="beryllium">4-Beryllium</option>
<option value="boron">5-Boron</option>
<option value="carbon">6-Carbon</option>
<option value="nitrogen">7-Nitrogen</option>
<option value="oxygen">8-Oxygen</option>

```

<option value="fluorine">9-Fluorine</option>  
<option value="neon">10-Neon</option>  
<option value="sodium">11-Sodium</option>  
<option value="magnesium">12-Magnesium</option>  
<option value="aluminum">13-Aluminum</option>  
<option value="silicon">14-Silicon</option>  
<option value="phosphorus">15-Phosphorus</option>  
<option value="sulfur">16-Sulfur</option>

<option value="chlorine">17-Chlorine</option>  
<option value="argon">18-Argon</option>  
<option value="potassium">19-Potassium</option>  
<option value="calcium">20-Calcium</option>  
<option value="scandium">21-Scandium</option>  
<option value="titanium">22-Titanium</option>  
<option value="vanadium">23-Vanadium</option>  
<option value="chromium">24-Chromium</option>  
<option value="manganese">25-Manganese</option>  
<option value="iron">26-Iron</option>  
<option value="cobalt">27-Cobalt</option>  
<option value="nickel">28-Nickel</option>  
<option value="copper">29-Copper</option>  
<option value="zinc">30-Zinc</option>  
<option value="gallium">31-Gallium</option>  
<option value="germanium">32-Germanium</option>

<option value="arsenic">33-Arsenic</option>  
<option value="selenium">34-Selenium</option>  
<option value="bromine">35-Bromine</option>  
<option value="krypton">36-Krypton</option>  
<option value="rubidium">37-Rubidium</option>  
<option value="strontium">38-Strontium</option>  
<option value="yttria">39-Yttria</option>  
<option value="zirconium">40-Zirconium</option>  
<option value="niobium">41-Niobium</option>  
<option value="molybdenum">42-Molybdenum</option>  
<option value="technitium">43-Technitium</option>  
<option value="rhodium">44-Rhodium</option>  
<option value="ruthenium">45-Ruthenium</option>  
<option value="rhodium">46-Rhodium</option>  
<option value="silver">47-Silver</option>  
<option value="cadmium">48-Cadmium</option>

<option value="indium">49-Indium</option>  
<option value="tin">50-Tin</option>  
<option value="antimony">51-Antimony</option>  
<option value="tellurium">52-Tellurium</option>  
<option value="iodine">53-Iodine</option>  
<option value="xenon">54-Xenon</option>  
<option value="cesium">55-Cesium</option>  
<option value="barium">56-Barium</option>  
<option value="lanthanum">57-Lanthanum</option>  
<option value="cerium">58-Cerium</option>  
<option value="praseodymium">59-Praseodymium</option>  
<option value="neodymium">60-Neodymium</option>  
<option value="promethium">61-Promethium</option>  
<option value="samarium">62-Samarium</option>  
<option value="europium">63-Europium</option>  
<option value="gadolinium">64-Gadolinium</option>

<option value="terbium">65-Terbium</option>  
<option value="dysprosium">66-Dysprosium</option>  
<option value="holmium">67-Holmium</option>  
<option value="erbium">68-Erbium</option>

```

<option value="thulium">69-Thulium</option>
<option value="ytterbium">70-Ytterbium</option>
<option value="lutetium">71-Lutetium</option>
<option value="hafnium">72-Hafnium</option>
<option value="tantalum">73-Tantalum</option>
<option value="tungsten">74-Tungsten</option>
<option value="rhenium">75-Rhenium</option>
<option value="osmium">76-Osmium</option>
<option value="iridium">77-Iridium</option>
<option value="platinum">78-Platinum</option>
<option value="gold">79-Gold</option>

<option value="mercury">80-Mercury</option>
<option value="thallium">81-Thallium</option>
<option value="lead">82-Lead</option>
<option value="bismuth">83-Bismuth</option>
<option value="polonium">84-Polonium</option>
<option value="astatine">85-Astatine</option>
<option value="radon">86-Radon</option>
<option value="francium">87-Francium</option>
<option value="radium">88-Radium</option>
<option value="actinium">89-Actinium</option>
<option value="thorium">90-Thorium</option>
<option value="protactinium">91-Protactinium</option>
<option value="uranium">92-Uranium</option>

```

```

</optgroup>
</select><br />

```

```
&<br>
```

```

Wavelength: <select class="fdd" id="fd3">
  <option value="Any">Any</option>
  <option value="785">785nm</option>
  <option value="532">532nm</option>

```

```
</select><br>
```

```
<a id="help" href="/html/help.html">Help</a>&nbsp;&nbsp;&nbsp;
```

```

</fieldset>
</div><br>

```

```

<form id="filersForm">
Please select a letter:&nbsp;&nbsp;&nbsp;

```

```

<span class="beta" value="A" shift="190" name="letter" >A</span>
<span class="beta" value="B" shift="190" name="letter" >B</span>
<span class="beta" value="C" shift="190" name="letter" >C</span>
<span class="beta" value="D" shift="190" name="letter" >D</span>
<span class="beta" value="E" shift="190" name="letter" >E</span>
<span class="beta" value="F" shift="190" name="letter" >F</span>
<span class="beta" value="G" shift="190" name="letter" >G</span>
<span class="beta" value="H" shift="250" name="letter" >H</span>
<span class="beta" value="I" shift="250" name="letter" >I</span>
<span class="beta" value="J" shift="250" name="letter" >J</span>
<span class="beta" value="K" shift="250" name="letter" >K</span>
<span class="beta" value="L" shift="250" name="letter" >L</span>
<span class="beta" value="M" shift="300" name="letter" >M</span>
<span class="beta" value="N" shift="300" name="letter" >N</span>

```

```

<span class="beta" value="O" shift="300" name="letter" >O</span>
<span class="beta" value="P" shift="400" name="letter" >P</span>
<span class="beta" value="Q" shift="400" name="letter" >Q</span>
<span class="beta" value="R" shift="400" name="letter" >R</span>
<span class="beta" value="S" shift="400" name="letter" >S</span>
<span class="beta" value="T" shift="480" name="letter" >T</span>
<span class="beta" value="U" shift="480" name="letter" >U</span>
<span class="beta" value="V" shift="480" name="letter" >V</span>
<span class="beta" value="W" shift="480" name="letter" >W</span>
<span class="beta" value="X" shift="580" name="letter" >X</span>
<span class="beta" value="Y" shift="580" name="letter" >Y</span>
<span class="beta" value="Z" shift="580" name="letter" >Z</span>

  or 

<span class="ui-widget" id="ac"><INPUT type="text"
id="tags"></input></span>&nbsp;&nbsp;&nbsp;<button id="tagsb"
type="submit">Search</button>&nbsp;&nbsp;&nbsp;

or

</form>

<span id="mspace"><button id="multip" type="submit" >Separate
Spectra</button></span>
<span id="mspace2"><button id="combin" type="submit" >Overlay Spectra
</button></span>
<button id="reload">Clear All</button>&nbsp;&nbsp;

<br><button id="loginb" >Log In</button>&nbsp;&nbsp;

<span id="login">Username:&nbsp;&nbsp;<input type="text"
id="loginu"></input>&nbsp;&nbsp;&nbsp;Password:&nbsp;&nbsp;&nbsp;
<input type="text" id="loginp"></input>&nbsp;&nbsp;&nbsp;<button id="logins"
type="submit">Submit</button><button type="submit" id="loginn">New
User</button></span><span id="loginr">Username:</span>
</div>

<div id="dl" style="overflow:auto;"></div>

<div id="header2" >

Mineral Name:&nbsp;&nbsp;<span id="mn"></span><br>
Alphabet:&nbsp;&nbsp;<span id="alp"></span><br>
Selected Filters:&nbsp;&nbsp;<span id="fil"></span><br>
Selected Spectra:&nbsp;&nbsp;<span id="gph"></span><br>
Filter Span:<span id="chem3"></span>

</div>
<div id="ip"></div>
<div id="activit"></div>
<div id="activita"></div>

<div id="holder">
  <div id="leftBar">

```

```

</div>

<div id="content">
Please select a spectra with the site utilities

</div>

<div id="footer">
<span class="text">&#169 2013 John F.Turner II. All rights reserved.

<span id="f2"><a id="csulink" href="http://www.csuohio.edu"
target="_blank">Cleveland State University</a></span></span>
</div>

```

```

</div>

```

```

<script>//for the filter selection area

```

```

$(document).ready(function(){

//var Me=3;
$('#tags').attr('value', "");
$('.ddc').attr('checked', false); //for startup
//$('#dd').attr('value', "");
var fill =[];

//Show hide list

$("#ddd").click(function(){

$("#df").toggle();

});

$("#df").mouseleave(function(){
$("#df").hide();
});

$(".sb").click(function(){

$("#df").show();

});

//Filter selection(new)

$('.fdd').change(function() {
//alert('Handler for .change() called.');
```

```

    $('#content').empty();
    $('#activita').show().ajaxStop(function(){
    $('#activita').hide();
    });

    var fd1=$("#fd1 option:selected").text();
    var fd2=$("#fd2 option:selected").text();
    var fd3=$("#fd3 option:selected").val();

```

```

    alert("Selected value 1: " + fd1);
    alert("Selected value 2: " + fd2);
    alert("Selected value 3: " + fd3);
    $('#leftBar').load('/html/ramindex_displaydb_filters2.php',{fd1: fd1,
fd2:fd2, fd3:fd3 });
});

$('.ddc').click(function(){
$(".fselected").each(function (i)
    {
        fill[i]=$ (this).attr("id");
    });

//$('#trigger').click(function(){

//var change = "new";

if ($(this).attr('checked')){
var fVal =$(this).next('span').attr("id");
var fcheck=jQuery.inArray(fVal, fill); //-1 or element
$("#chem").text(fcheck);
$("#chem2").text(fVal);
}

if (fcheck!=-1){
    //alert("The filter has been removed");

    var removeitem = $(this).next('span').clone().text();
    //alert(removeitem);
    $("#fil :contains("+removeitem+")").remove();
    fill.splice( $.inArray(fcheck, fill), 1 );

    $("#chem").text(fcheck);
    //$("#chem2").text(fVal);
    //$("#chem2").html(removeitem);

var fMe=$('#fil').text();

$("#chem3").text(''+fMe+'');
var fMe=$('#chem3').text();

//$('#ddd').html('');
$('#ddd').html('<input id=dd value='+fMe+'></input>');

    }

if (fcheck==--1){
$('#fil').append($(this).next('span').clone().addClass("fselected").appe
nd(", "+" "));

//$('#fil').append(", "+" ");

var fMe=$('#fil').text();

$("#chem3").text(''+fMe+'');
var fMe=$('#chem3').text();

//$('#ddd').html('');
$('#ddd').html('<input id=dd value='+fMe+'></input>');

```



```
}

//$('#change').html(function() {
    //var line='<input value='+change+ '></input>';
    //return line;
//});
});
});

$(".beta").click(function(){
    //$("#dl").hide();
    $("#dl").show();
});

</script>
```

## APPENDIX M:

### Ramindex database search “fetchCriteria2.php”

```
<?php
$min=$_GET['term'];

//echo $min;
//$min='barylite';

$Host = "██████████";
>User = "██████████";

>Password = "██████████";

$sql = "██████";
//$TableName = "██████████";
$TableName = "██████████";

$link = mysql_connect($Host, $User, $Password);
if (!$link) die("Unable to connect to MySQL: " . mysql_error());

$db_selected = mysql_select_db($sql, $link);
if (!$db_selected) {
    die ("Can't use $sql : " . mysql_error());
}

$query=mysql_query("SELECT MineralName from $TableName WHERE MineralName
REGEXP '^$min'") ;

//$result= mysql_query($query);

//$row = mysql_fetch_array($query) or die(mysql_error());
//echo $row;

while ($row = mysql_fetch_array($query)) {
    $data[] = trim($row[0]);
}
//print_r ($data);

//print_r($row);

//foreach($row as $v){
    //echo $v;
//}

echo json_encode($data);
//print_r($data);
//mysql_free_result($result);
mysql_close($link);

?>
```

## APPENDIX N:

### Ramindex display search results “ramindex\_displaydb31.php”

```
<link rel="icon" href="/html/images/RamIndexIcon.ico" type="image/x-
icon"/>
<link rel="shortcut icon" href="/html/images/RamIndexIcon.ico"
type="image/x-icon"/>

<?php //PHP part only displays the found items. This is where multiple
data can be shown

//$mmineralname=array('this','is','crazy','');
//print_r($mmineralname);
//$ccount=count($mmineralname);
//echo $ccount;
//$splice_count=$ccount-1;
//echo $splice_count;
//$iinputs = array_splice($mmineralname,0,$splice_count);
//print_r($iinputs);

//$countinputs=count($iinputs);
//echo $countinputs;

$mineralname=$_REQUEST['mineralname'];

//Check to condition of comma at the end
//echo strlen($mineralname);
//$last=substr($mineralname, strlen($mineralname)-2, 1);
//echo $last;

//Add comma to process if not at end
//if($last!=""){
//$mineralname=$mineralname.", ";
//echo $mineralname;

//} //End of if", " condition

$inputs = explode(", ", $mineralname);
$ninputs=array_map("trim",$inputs); //Trims the whitespace off the
begining of
//echo $inputs;

$ninputs=array_filter($ninputs);//Remove unset keys
$zninputs=array_values($ninputs);//Resest the key order
//print_r ($zninputs);

//Check for unique values
$result = array_unique($zninputs);
//print_r($result);

//Check array from repetitions; convert string to lower

//foreach($result as $key=>$value){
//echo "$value<br>";

//for($ct=0;$ct<=2; $ct++){
//$found=strcasecmp($value , $result[$ct] );
//if(strcasecmp ($value, $result[$ct])==0) {
```

```

//echo "<br>$ct";
//echo "<br>$value";
//echo $key;

//if($ct!=$key){
//echo "Delete Me $key";
//}
//}

$r = array_intersect_key($result, array_unique(array_map('strtolower',
$result)));
$fr=array_values($r);//Resest the key order
//print_r($r);

//String match each key value, find position of match, delete them,
filter new search array

//$count=count($ninputs);
//echo ($count);
//echo ("Mineral count is: ".$count-1);

//if ($count>=2){
//$newname=substr($mineralname,0,-2);
//echo $newname;
//}

//else{

//echo $mineralname;
//}

//Arrays multiple inputs

//$arraycount=count($zninputs);
$arraycount=count($r);
//echo $arraycount;
//print_r($zninputs);

//if (mineralname[$arraycount-1]==""){
//$arraycount=$arraycount-1;
//echo $arraycount; //The number of samples
//}
//end

//echo $arraycount;
//echo $inputs[0]; // piece1
//echo $inputs[1]; // piece2
//echo $inputs[2]; // piece3
//echo $inputs[3];

//$filters=$_REQUEST['filters'];

//echo $filters;

$Host = "██████████";
$User = "██████████";
$Password = "██████████";

```

```

$sql = "██████";
$TableName = "██████";

$link = mysql_connect($Host, $User, $Password);
if (! $link) die("Unable to connect to MySQL: " . mysql_error());

$db_selected = mysql_select_db($sql, $link);
if (!$db_selected) {
    die ('Can\'t use $sql : ' . mysql_error());
}

$j=0; //Count for the pagination
//echo $j;

if(!empty($mineralname)){

    //$i=2; //test iteration
    //echo $ninputs[$i];

    //echo "$mineralname";

    for ($i=0;$i<$arraycount;$i++){

        //echo $i."Thenumber";
        //echo $zninputs[$i];

        $Query = sprintf("SELECT * from $TableName WHERE MineralName Like
'$fr[$i]' OR Sample Like '$zninputs[$i]'");
        // $mineralname used previous
        $Result = mysql_query ($Query,
            $link) ;

        //echo $Result;

        $num_rows = mysql_num_rows($Result);

        //echo $num_rows;

        //echo "$num_rows Rows\n"; Show # of rows matched

        //$nresult="$Result";
        //echo $nresult;
        if($num_rows ==0){
            echo "$zninputs[$i] no data<br>";
        }

        //echo "$ninputs[$i]";

        //$Row = mysql_fetch_array($Result); Use for single fetch for Name only
        //print_r($Row);
        //echo "$Row[MineralName]";

        while ($Row = mysql_fetch_array($Result)){

            //echo $Row;
            //$Row = mysql_fetch_array($Result);

            //$nresult="$Row[MineralName]";
            //echo "$nresult";
        }
    }
}

```

```

//print_r($Row);

if (isset($Row['0'])) {
//echo "set";
//echo "$Row[Sample]";

$query2 = sprintf("SELECT * from sdata WHERE cook Like '$Row[Sample]'");
//For data

$result2 = mysql_query ($query2,
$link) ;//For data
$rowdata=mysql_fetch_array($result2);
//echo "$Rowdata[0]"; //Show if exists
//echo "set";

if(isset($rowdata['0'])){
//echo ("here");
//echo "<input class=item type=checkbox id=$Row[Sample]
mns=$Row[MineralName]></input><a
//href=\"mineral_dataform11.php?mineralname=$Row[MineralName]&nbsp;&cook=
$Row[Sample]\" //alt=\"altText\"
name=\"mineralname\">$Row[MineralName]</a>&nbsp;$Row[Sample]<br> " ;

echo "<input class=item type=checkbox id=$Row[Sample]
mns=$Row[MineralName] ></input><a
id=$Row[Sample] mns=$Row[MineralName] class=cn
href=\"mineral_dataform13.php?mineralname=$Row[MineralName]&cook=$Row[Sample]\" target=\"_blank\">$Row[MineralName]</a><span
id=$Row[Sample]>&nbsp;$Row[Sample]</span><br> " ;

}

}

//} //Here is what is sent to left bar.

if(!isset($rowdata['0'])){

echo "$fr[$i] $Row[Sample] no data\n <br>";

}
} //For the while loop;

}

}

?>

<title>jQuery pagination</title>

<!--Javascript Library Files -->
<script src="/html/jquery-1.7.1.js"></script>
<script src="/html/jquery/js/jquery-ui-1.8.16.custom.min.js"></script>

<script type=text/javascript>

var alertflag=0;

//Set all items to true from the initial search per Dr.T

```

```

//Page initialization script below

$(function(){

$('#leftBar :input').attr('checked', true);

});

var graphspectra=[];
var gspecnames=[];

//$('#tes').click(function(){

//alert("The # of inputs is: " +$('#leftBar :input').size());

$('#leftBar input').each(function(index){

    graphspectra[index]=$ (this).attr("id");
    gspecnames[index]=$ (this).attr("mns")+" "+$(this).attr("id");
    //alert(graphspectra[index]);
    //alert($(this).attr("mns")); //Use for the series names

});

//Append the Cook number to selected spectra
$.each(graphspectra, function (i,cn)
    {

        //alert("Append cook: " +cn);
        $('#gph').append(graphspectra[i]).append(", "+" ");
        //graphspectra[i]=$ (this).attr("id");

    });

//});

//alert(graphspectra[0]);

var e=graphspectra.length; //From the above automation
//alert(e);

$('#content').load('/html/highchart101.html', {spectra:graphspectra,
names:gspecnames});
//alert(graphspectra.length);
//Page working section below
//alert(e);

$('.item').click(function(){

$('#combin2').remove();
$('#multip').remove()

//alert($(this).attr("id"));

//var ani=3;
//var bw=5;
//var ZZv="B";
var graphVal=$(this).attr("id");
var graphcheck=jQuery.inArray(graphVal, graphspectra); //-1 or element
//alert(graphspectra.length);

//alert(graphcheck);

//Section for removing selected spectra from the array

```

```

if (graphcheck!=-1){
    //alert("The sampple has been selected");

    //alert("The spectra has been removed");
    //var remspecitem = $(this).next('span').clone().text();
    var remspecitem = $(this).next('span').attr("id");

if (alertflag==1){
    alert("remove:"+remspecitem);
}
    //alert(remspecitem);
    //$("#gph :contains("+remspecitem+")").remove(); //good
    //$("#gph :contains("remspecitem")").remove();
    //$("#chem4 :contains("+remspecitem+")").remove();
    //$("#chem4").empty();
    //alert("graphcheck:" +graphcheck);
    //alert("graphspectra before:" +graphspectra);
    //alert("array position:"+graphcheck);
    graphspectra.splice( graphcheck, 1 );
    //alert("graphspectra after:" +graphspectra);
    //alert("graphspectra new size: "+graphspectra.length);

//Replace with new text for selected spectra

    //if (graphcheck==0){
        $('#gph').empty();
    //}
    $.each(graphspectra, function (i,cn)
    {

if (alertflag==1){
    alert("new: "+cn);

}

        $('#gph').append(graphspectra[i]).append(", "+" ");
        //graphspectra[i]=$ (this).attr("id");
    });

    //$("#chem").text(graphcheck);
    //$("#chem2").text(fVal);
    //$("#chem2").html(removeitem);

var gMe=$('#graphspectra').text();

    //$("#chem3").text(''+gMe+'');
    //var gMe=$('#chem3').text();

    //$("#ddd").html('');
    //$("#ddd").html('<input id=dd value='+gMe+'></input>'); //For adding to
input for filter

e=e-1;

if (alertflag==1){
    alert("e:" +e);
}

//Update labels

if (alertflag==1){
    alert("gspecnames before:" +gspecnames);
}

```



```

}

gspecnames.splice( graphcheck, 1 );

if (alertflag==1){
alert("gspecname after:" +gspecnames);
}

$('#content').load('/html/highchart101.html', {spectra:graphspectra,
names:gspecnames});
}

if ($(this).attr('checked') ){ //Hooray!! 1 day to get right; works
at .ere level

//Create an array with a index value from php, or jquery us index value
to alert if selected

//If they go to remove should I ask if they really want to remove?(no
for now)

    //var graphVal =$(this).next('span').attr("id");
    //var graphVal =$(this).attr("id");

//alert(graphVal);

    //var graphcheck=jQuery.inArray(graphVal, graphspectra);
//alert(graphcheck);

if (graphcheck==-1){

    //$(this).addClass(".gselected");
//alert(graphspectra.length);

graphspectra[e]=$(this).attr("id");

if (alertflag==1){
alert("graphspectra:"+graphspectra.length);

alert(graphspectra);
}

e++;

if (alertflag==1){
alert("e:"+e);
}

    //alert(graphspectra.length);
//run the search function with name of the mineral; return the append
results to the //leftbox

//Need to make an array to scan for item removal or use replace string

    //alert($(this).attr("mns"));

$('#gph').append($(this).next('span').clone().addClass("gselected").appe
nd(", "+" "));
//$('#gph').append($(this).next().next('span').clone().addClass("gselect
ed"));

```

```

//var mid=$(this).attr("id");
//alert(mid);
//$('#gph').append(mid);

$(".gselected").each(function (i,cn)
{
    //alert("cn: "+cn);
    //graphspectra[i]=$(this).attr("id");
});
$.each(graphspectra, function (i,cn)
{
    //alert("Here2");
    //alert(cn);
    //graphspectra[i]=$(this).attr("id");
});

//alert($(this).next('span').text());
//$("#content2").html(graphVal); Keep as diagnostic

//$("#span:contains('Zinc')").css("text-decoration", "underline");
//works

//$('#gph').append(", "+" ");

var gMe=$('#gph').text(); //trim();
$('#chem4').text(''+gMe+'');
//$("#tags").attr('value', gMe);

}
if (alertflag==1){
alert("gspecnames before:" +gspecnames);
}

gspecnames.push( $(this).attr("mns")+" "+$(this).attr("id") );

if (alertflag==1){
alert("gspecname after:" +gspecnames);
}

$('#content').load('/html/highchart101.html', {spectra:graphspectra,
names:gspecnames}); //mdata8.html

//alert(graphspectra.size);
}

});
//});

</script>

<script>

$(".cn").mouseover(function(){
$("#ip").show();

//alert($(this).attr("id"));

cook=$(this).attr("id");
//alert(cook);
var mineralname=$(this).attr("mns");

```

```

var position = $(this).offset();
//console.log(position);

for(var key in position) {
    //alert('key: ' + key + '\n' + 'value: ' + position[key]);
}
//alert(key);
//alert(position[key]);
//alert(position["top"]);

//var shift = $(this).attr("shift");
//$("#alp2").text(shift);

//$("#ip").css("margin-left", shift+"px");
$("#ip").css("margin-left", 140+"px");

//alert("help");
//alert(position["top"]);
$("#ip").css("margin-top", (position["top"]-270)+"px");

//Load the images for the samples
$('#ip').load('/html/flyout_min_images2.php',{mineralname: mineralname,
cook:cook});

    $('#ip').mouseleave(function(){
        $('#ip').hide();

    });

$('#*').click(function(){
    $('#ip').hide();

    });

});

//Highlights the anchors
$(".cn").hover(function(){
    $(this).css("background", "red");
    $(".cn").mouseout(function(){
        $(".cn").css("background", "none")
    });
});
</script>

```

## APPENDIX O:

### Highcharts plug-ins needed

#### Ramindex chart display “highchart101.html”

```
<!DOCTYPE html PUBLIC "-//W3C//DTD XHTML 1.1//EN" "xhtml11.dtd">

<html debug="true">
<head>
<title>Highcharts Demo Gallery</title>
<meta http-equiv="Content-Type" content="text/html; charset=utf-8" />
<!-- meta http-equiv="X-UA-Compatible" content="chrome=1" -->

<link rel="icon" href="/html/images/RamIndexIcon.ico" type="image/x-
icon"/>
<link rel="shortcut icon" href="/html/images/RamIndexIcon.ico"
type="image/x-icon"/>

<script src="/html/jquery-1.7.1.js"></script>
<script src="/html/jquery/js/jquery-ui-1.8.16.custom.min.js"></script>

<script type="text/javascript"
src="http://ajax.googleapis.com/ajax/libs/jquery/1.7.1/jquery.min.js"></
script>
<script type="text/javascript">
jQuery.noConflict();
</script>

<!-- Highslide code -->
</script type="text/javascript" src="/highslide/highslide-
full.min.js"></script>
</script type="text/javascript" src="/highslide/highslide.config.js"
charset="utf-8"></script>
<link rel="stylesheet" type="text/css" href="/highslide/highslide.css"
/>
<!--[if lt IE 7]>
<link rel="stylesheet" type="text/css" href="/highslide/highslide-
ie6.css" />
<![endif]-->
<!-- End Highslide code -->

<script type="text/javascript">
var example = 'line-basic',
    theme = 'default';
</script>

</script type="text/javascript" src="/demo/scripts.js"></script>

<link rel="stylesheet" href="/templates/yoo_symphony/css/template.css"
type="text/css" />
<link rel="stylesheet"
href="/templates/yoo_symphony/css/variations/brown.css" type="text/css"
/>
<link href="/demo/demo.css" rel="stylesheet" type="text/css" />

<script type="text/javascript">

//Show and give separate button functionality with toggle feature
```

```

$(document).ready(function(){
//alert(" highchart loaded");
$('#combin').remove();
$('#combin2').remove();

$('#multip').remove();

$('#mspace').append("<button id=multip type=submit>Separate Spectra</button>");

$('#multip').click(function(){
//alert("multip clicked");

$('#content').load('/html/highchart20multi.html');
//$('#content').load('/html/test1.html');
$('#combin').remove();
$('#multip').hide();
$('#mspace2').append("<button id=combin2 type=submit>Overlay Spectra</button>");

//$('#combin2').show();
$('#combin2').click(function(){

$('#content').load('/html/highchart101.html',
{spectra:graphspectra});
$('#combin2').remove();
});

//$('#combin2').show();
//$('#*').unbind();
});

if (graphspectra.length>=2){
$('#multip').show();
}

//else{
//$('#multip').hide();
//}

});

//Get the size of graph spectra
//var graphspectra=["C0475","C0476"];
//alert(graphspectra.length);
//data1=[1, 8, 4];

```

```

//alert(graphspectra);
//alert(gspecnames); //Name for each spectra

(function($){ // encapsulate jQuery

//graphspectra="C0597";//spectra:graphspectra,

var options={
chart: {
    renderTo: 'containe',
    type: 'line',
    zoomType: 'x',
    //lineWidth:0.5,
    shadow:false

    },

title: {
    text: 'Raman Spectra'
    },

plotOptions: {
    series: {
        lineWidth:1,
        shadow:false,
        marker: {
            radius: 0
        }
    }
    },

tooltip: {
    crosshairs: {
        color: 'green',
        dashStyle: 'solid'
    },
    shared: true
    },

yAxis: {
    title: {
        text: 'Intensity (counts)'
    },

labels: {
formatter: function() {
    return this.value
    }
    },

xAxis: {

    title: {
        enabled: true,
        text: 'Raman Shift (cm<sup>-1</sup>)'
    }

    },
},

```

```

        series: []
    }

$.getJSON('/html/fetchSpectral10.php', { spectra:graphspectra,
mdata:'new'},function(res) {

for (i in res){

//alert(res[i]);
//alert(i);

//data1=[];

//alert(res);
//alert(res.split(','));
//alert($.trim(res));
//alert(JSON.parse(res));

//var i=0;
//alert(gspecnames[i]);

x="data"+i;
    //alert(x);

    x={

        name: gspecnames[i],

        data:[]

    }

$.each(res[i], function(itemNo, item) {
    //alert(item);

//jQuery.each(item, function() {
    //alert(parseInt(item));
    //});

//Section for adding series
//i=0;

    //x="series"+i;
    //x = {
        //data: []

        //};
    //$.each(s1, function(itemNo,iplot){
    //alert(iplot);

    //alert(x);

    //x.data.push(parseFloat(iplot)); //Plot
    //x.data.push(parseFloat(iplot)); //Plot
    x.data.push(parseFloat(item)); //Plot
    //i++;
    //});

//alert(item);
    //data1.push(item);

```

```

        //data1.push(parseFloat(item)); //parseFloat changes
from str to //num!!Very important!!
    });

options.series.push(x);
}

var chart1; // globally available
$(document).ready(function() {
    chart1 = new Highcharts.Chart(options);
$('#leftBar').height($('#content').height()+2);
});
})(jQuery);
</script>

</head>
<body>

<div id="demo-content">
    <div style="margin: 0 1em">
        <script src="/html/highcharts/js/highcharts.js"></script><script
src="http://code.highcharts.com/modules/exporting.js"></script>

<div id="containe" style="width: 760px; height: 500px; "></div>
    <div style="margin: 1em">

        <div class="buttons">
            <div class="highslide-maincontent">
                </div>
            </div>
        </div>
    </div>

</div>

</body>

</html>

```



## APPENDIX P:

### Ramindex multicharts “highchart20multi.html”

```
<!DOCTYPE html PUBLIC "-//W3C//DTD XHTML 1.1//EN" "xhtml11.dtd">

<link rel="icon" href="/html/images/RamIndexIcon.ico" type="image/x-
icon"/>
<link rel="shortcut icon" href="/html/images/RamIndexIcon.ico"
type="image/x-icon"/>

<html debug="true">
<head>
<title>Highcharts Demo Gallery</title>
<meta http-equiv="Content-Type" content="text/html; charset=utf-8" />
<!-- meta http-equiv="X-UA-Compatible" content="chrome=1" -->

<script src="/html/jquery-1.7.1.js"></script>
<script src="/html/jquery/js/jquery-ui-1.8.16.custom.min.js"></script>

<script type="text/javascript"
src="http://ajax.googleapis.com/ajax/libs/jquery/1.7.1/jquery.min.js"></
script>
<script type="text/javascript">
jQuery.noConflict();
</script>

<!-- Highslide code -->
</script type="text/javascript" src="/highslide/highslide-
full.min.js"></script>
</script type="text/javascript" src="/highslide/highslide.config.js"
charset="utf-8"></script>
<link rel="stylesheet" type="text/css" href="/highslide/highslide.css"
/>
<!--[if lt IE 7]>
<link rel="stylesheet" type="text/css" href="/highslide/highslide-
ie6.css" />
<![endif]-->
<!-- End Highslide code -->

<script type="text/javascript">
var example = 'line-basic',
    theme = 'default';
</script>

</script type="text/javascript" src="/demo/scripts.js"></script>

<link rel="stylesheet" href="/templates/yoo_symphony/css/template.css"
type="text/css" />
<link rel="stylesheet"
href="/templates/yoo_symphony/css/variations/brown.css" type="text/css"
/>
<link href="/demo/demo.css" rel="stylesheet" type="text/css" />

<script>
//alert("here");
</script>
```

```

<script type="text/javascript">
$(document).ready(function(){

//alert("Number graph containers: "+ graphspectra.length);

//
//$('#combin').hide();
if (graphspectra.length>=2){
//$('#combin2').show();
}
else{
//$('#multip').hide();
}
});

//Get the size of graph spectra
//var graphspectra=["C0475","C0597"];
//alert(graphspectra.length);
//data1=[1, 8, 4];

//alert(graphspectra);
//(function($){ // encapsulate jQuery
//graphspectra="C0597";//spectra:graphspectra,

$.getJSON('/html/fetchSpectral10.php', {spectra:graphspectra,
mdata:'new'},function(res) {

var d="0";

for(gc=0;gc<graphspectra.length;gc++){

//alert(gc);

$('#h1').append("<span class=sps id=container"+gc+">here</span><br>");
}

for (i=0;i<gc;i++){

var options={
chart: {
renderTo: 'container'+d,
type: 'line',
zoomType: 'x',
//lineWidth:0.5,
shadow:false

```

```

        },
title: {
    text: 'Raman Spectra'
},

plotOptions: {
    series: {
        lineWidth:1,
        shadow:false,
        marker: {
            radius: 0
        }
    }
},
yAxis: {
    title: {
        text: 'Intensity (counts)'
    }
},

},

labels: {
formatter: function() {
    return this.value
}
},

xAxis: {

    title: {
        enabled: true,
        text: 'Raman Shift (cm<sup>-1</sup>)'
    }

},
    series: []
}

var x=[];

x[i]={
    name: gspecnames[i],
    data:[]
}

//alert("Number is: "+i);

var co=[];
//co[i]=options;

```

```

//alert("counter is : " +d);

$.each(res[d], function(itemNo, item) {
    //alert(item);

    //jQuery.each(item, function() {
        //alert(parseInt(item));
    //});

    //Section for adding series
    //i=0;
        //y="series"+i;
        //x = {
            //data: []

            //};
        //$.each(s1, function(itemNo, iplot){
        //alert(iplot);

        //alert(x);

        //x.data.push(parseFloat(iplot)); //Plot
        //x.data.push(parseFloat(iplot)); //Plot
        x[i].data.push(parseFloat(item)); //Pushes on at a
time
        //i++;
        //});

        //alert(x);
        //data1.push(item);
        //data1.push(parseFloat(item)); //parseFloat changes
from str to //num!!Very important!!

    });

var g=i;
//alert("Number still is: " +g);
options.series.push(x[i]);
//alert("Set: "+g+" loaded");
d++;
var chart1; // globally available
chart1 = new Highcharts.Chart(options);

}

//alert($('#content').height());
$('#leftBar').height($('#content').height()+2);

});
//})(jQuery);

</script>

</head>

<body>

```

```
<div id="demo-content">
  <div id="h1" style="margin: 0 1em">
    <script
src="/html/highcharts/js/highcharts.js"></script><script
src="http://code.highcharts.com/modules/exporting.js"></script>

  </div>
  <div style="margin: 1em">

    <div class="buttons">
      <div class="highslide-maincontent">
        </div>
      </div>
    </div>
  </div>

</div>
</body>
</html>
```

## APPENDIX Q:

### Ramindex locate spectra “fetchSpectra10.php”

```
<?php
//$spectra=array("C0597","C0475");

$minid=$_GET['spectra'];
//echo $minid;
//print_r ($minid);
//print_r($minid);
//$min=$_GET['mdata'];
$ir=count($minid);
//echo $ir;
//$min=array(1,2);
//$ginputs = explode(",", $minid);
//$ginputs = explode(",", $spectra);
//$nginputs=array_map("trim",$minid);
//echo $nginputs[0];
//echo "<br>";

$Host = "██████████";
>User = "██████████";

>Password = "██████████";

$sql = "██████";
//$TableName = "██████████";
$TableName = "██████████";
$TableName5="██████";

$link = mysql_connect($Host, $User, $Password);
if (! $link) die("Unable to connect to MySQL: " . mysql_error());

$db_selected = mysql_select_db($sql, $link);
if (!$db_selected) {
    die ("Can't use $sql : " . mysql_error());
}

//$i=0;
for ($i=0;$i<$ir;$i++){
//echo $i;
$query = sprintf("SELECT data from $TableName5 WHERE
cook='$minid[$i]');
//$minid[$i] or $minid
//$query = sprintf("SELECT arraydata from $TableName5 WHERE
cook='C0597'");

$result = mysql_query ($query,
$link) ;

$row = mysql_fetch_array($result);
//print_r ($row);
$datay1 = explode(",", $row[0]);
//$datay1=$row[0];
```

```

if ($i==0){
//$res=array($row); //$row[0];
//$res=$row;
$res=array($datay1);
//$res=$datay1;
//$res[0]=$row[0];

//$res=implode(",", $res);

//echo $res;
//print_r($res);

}

//$datay[0]=$row[0];
//$datay[0]="600,400,500";
//$datay[1]="450,500,610";
//$res=array($datay1,$datay[1]);

//$res=array(4,2);
//$ress=str_split($res);

if($i>=1){
//print_r($datay1);
array_push($res, $datay1); //$row[0]

//echo $row[0];
//$datay2=explode(",", $row);
//echo $datay2;
//$res[1]=datay2;
//$res=implode(",", $res);
//var_dump(
//    $res,
//    json_encode($res)
//);
}

}
//echo $res;
//$datay1="me";

echo json_encode($res);
//echo json_encode($datay1);
//mysql_close($Link);
?>

```

## APPENDIX R:

### Ramindex drop down list “cbox7.php”

```
<meta
http-equiv="content-type" content="text/html;
charset=encoding" />

<link rel="icon" href="/html/images/RamIndexIcon.ico" type="image/x-
icon"/>
<link rel="shortcut icon" href="/html/images/RamIndexIcon.ico"
type="image/x-icon"/>

</link rel="stylesheet" type="text/css" href="/html/font_stylesheet.css"
/>
</link rel="stylesheet" type="text/css" href="/html/ri_margin.css" />

<?php
$Host = "██████████";
$User = "██████████";
>Password = "██████████";
$sql = "██████";
$TableName = "██████████";

$link = mysql_connect($Host, $User, $Password);
if (! $link) die("Unable to connect to MySQL: " . mysql_error());

$db_selected = mysql_select_db($sql, $link);
if (!$db_selected) {
    die ("Can't use $sql : " . mysql_error());
}

$letter=$_REQUEST['aletter'];

//$letter='b';
//echo $letter;

$query = ("SELECT * from $TableName WHERE Mineralname Like '$letter%'
");

$result = mysql_query ($query,
    $link) ;

$count = 0;
$max = 20;

while ($row = mysql_fetch_array($result) ) {

$count++;

//echo "$row[id]";

echo "<div class=rear >";

$trimmedRow=trim("$row[Mineralname]");
```



```

echo "<input class=ere type=\"checkbox\" /><span
id=$Row[id]>$trimmedRow</span> ";

echo "</div>";

}

?>

<!--<div class="rer">

<input type="checkbox" checked="checked" class="er"></input>
This is the spotsdfs
sfas
</div>

<div id="content">
Add here
</div>

<div id="content2">
<span>Text Area</span>
</div>

<input type="checkbox" checked="checked" class="er"></input>-->

<!--Javascript Library Files -->
<script src="/html/jquery-1.7.1.js"></script>
<script src="/html/jquery/js/jquery-ui-1.8.16.custom.min.js"></script>

<script type=text/javascript>
var alertflag=0;

$(document).ready(function(){
var ids =[];

//$('.er').attr('checked',false);
//$('.er').attr('checked',false);
//$('.rear').click(function(){
$('.ere').click(function(){

var an=3;
var b=5;
var ZZ="B";

$(".selected").each(function (i)
{
ids[i]=$ (this).attr("id");
});

```

```

if ($(this).attr('checked') ){ //Hooray!! 1 day to get right; works
at .ere level

//Create an array with a index value from php, or jquery us index value
to alert if selected

//If they go to remove should I ask if they really want to remove?(no
for now)

    //$("#content").html("<p>A is equal to B</p>");
    //var aSee =$(this).next('span').text().trim();
    var aVal =$(this).next('span').attr("id");

    //$("#content2").append($(this).next('span').text());
    //$("#content2").html(aSee);
    //$("#content2").html(aVal);

    //var $spans = $("span");
    //$spans.eq(0).text(jQuery.inArray(aVal, ids));
    var check=jQuery.inArray(aVal, ids);
    //$spans.eq(1).text(check);

if($('#tags').val()){

    var scheck=$(this).next('span').text();

if (alertflag==1){
    alert ("Picked: "+ scheck);
}
    var crosscheck=$('#tags').val(); //For crosscheck typed and cbox
values

if (alertflag==1){
    alert("Crosscheck value: " +crosscheck);
}

var patt1=new RegExp(scheck,"i");
//alert(patt1.test(crosscheck));

    var clength=crosscheck.length;

if (alertflag==1){
alert("Value: "+ crosscheck.length);

}

    var cnew=clength-1;

if (alertflag==1){
    alert("Value-1: "+cnew);

    alert("Comma check:" +crosscheck.charAt(cnew));

    alert("Comma check-1:" +crosscheck.charAt(cnew-1));
}

    var last=crosscheck.charAt(cnew);

if (alertflag==1){
    alert("Last character: "+last);
}

```

```

        var cc=(patt1.test(crosscheck));
if (alertflag==1){
    alert("Crosscheck result: "+ cc);
}

    if(cc==true){
if (alertflag==1){
    alert("Already typed: " +scheck);
}

        }
}

if (check!==-1){
    alert("The sample has been selected");
}

if (check===-1){

//run the search function with name of the mineral; return the append
results to the //leftbox

//Need to make an array to scan for item removal or use replace string
var em=$('#tags').val();

if(!em){
    //alert("No value in input");
    $('#mn').append($(this).next('span').clone().addClass("selected"));
}

    if(em){
        //alert("I have a value");
        $('#tags').val(""); //Clear #tags
        //$('#mn').append(", "+" ");
    }

if(cc!=true){
    //alert("not True");

    if(last!=","){
        //alert("Comma");
        $('#mn').append(",");
        //$('#tags').val($('#mn').text());
    }
    $('#mn').append($(this).next('span').clone().addClass("selected"));
}

    }

    //else{
    //$$(this).children('span').clone().appendTo('#test2');
    //$$(this).children('span').clone().appendTo('#results');
    //$$(this).children('span').clone().appendTo('#content');
    //$$('#content').append($(this).children('span').clone());
    //$$('#mn').append($(this).next('span').clone().addClass("selected"));
    //$$('#mnn').append($(this).next('span').clone().addClass("selected"));
}

```

```

//alert($('#mn').append($(this).next('span').clone().addClass("selected"
));
//$(this).appendTo('#content');
//$("#content2").html(aVal); Keep as diagnostic

//$("#span:contains('Zinc')").css("text-decoration", "underline");
//works

//$('#mn').append(", "+" ");

//$('#mnn').append(", "+" ");
//var Me = $(this).children('span').clone().text();
var Me = $('#mn').text(); //trim();
//alert(Me);
//$('#chem4').text(''+Me+'');

//Make a more sophisticated addition

//var tset=$("#tags").attr('value');
//alert($("#tags").attr('value'));
//alert(tset.toSource());

//Check to see if a value exist, then append the value to the input box

//alert(tset)

$("#tags").val(function(i, val) {
//$("#tags").empty();
//alert(tset)
//val=tset+", "+Me;
val=Me;
return val;
});

//$("#tags").attr('value', Me);

}

//if($("#div:contains('Add')")){

//$('#div :contains('aSee')').css("text-decoration",
"underline");
//$("#content2").text(aSee);

//}

}

//else {
//if (!$ (this).attr('checked') ){

// For removing from ids and later remove from selected class and mn
list
// var removeMe;
// $.each( myArray, function(i, v) {
//     if( v.name == 'Jim' ) {
//         removeMe = i;
//     }
// });
// myArray.splice(removeMe,1);

```

```
//else find see span and delete it
    //$("#content").html("<br><p>B is equal to A</p>");
    //}
//}

});
});

</script>
```

## APPENDIX S:

### Ramindex Splash Screen "index.html"

```
<title> RamIndex - a standardized spectral database</title>

<link rel="icon" href="/html/images/RamIndexIcon.ico" type="image/x-
icon"/>
<link rel="shortcut icon" href="/html/images/RamIndexIcon.ico"
type="image/x-icon"/>

<script src="/html/jquery-ui-1.10.1.custom/js/jquery-1.9.1.js"></script>
<script src="/html/jquery-ui-1.10.1.custom/js/jquery-ui-
1.10.1.custom.min.js"></script>
<link rel="stylesheet" type="text/css" href="/html/jquery-ui-
1.10.1.custom/css/dark-hive/jquery-ui-1.10.1.custom.css"/>

<script>

$(document).ready(function() {

function cycleImages(){
    var $active = $('#holder1 .active');

    var $next = ($active.next().length > 0) ? $active.next() :
$('#holder1 img:first');
    $next.css('z-index',2);//move the next image up the pile
    $active.delay(3000).fadeOut(2000,function(){//fade out the top
image
        $active.css('z-index',1).show().removeClass('active');//reset
the z-index and unhide the image
        $next.css('z-index',3).addClass('active');//make the next
image the top one
        cycleImages();
    });
}

cycleImages();

$(".beta").hover(function(){
    $(this).css("color","#659CC9"); //70A7D4
    $(".beta").mouseout(function(){
        $(".beta").css("color","#ffffff")
    });
});

//Directs the page to the Updates page

$('#updates').click(function(){

    //window.location = '/html/updates.html';
    alert("No updates are available at this time.");

});
```

```

//Directs the page to the Updates page

$('#projects').click(function(){
    //window.location = '/html/updates.html';
    //alert("Sorry, this area is still underdevelopment.");

var url = $(this).attr('href');
window.open('http://facultyprofile.csuohio.edu/csufacultyprofile/detail.cfm?FacultyID=J_F_TURNER', '_blank');

});

//Directs the page to the search page

function redirect() {
    window.location = '/html/test28.html';
}

$('#search').click(function(){
    redirect();
});

//Directs the page to the about page

$('#about').click(function(){
    //window.location =
'http://facultyprofile.csuohio.edu/csufacultyprofile/detail.cfm?FacultyID=J_F_TURNER';
    //alert("Sorry, this area is still underdevelopment.");

var url = $(this).attr('href');
window.open('http://facultyprofile.csuohio.edu/csufacultyprofile/detail.cfm?FacultyID=J_F_TURNER', '_blank');

});

//Directs the page to the contacts page

$('#contact').click(function(){
    //window.location = '/html/about.html';
    alert("Sorry, this area is still underdevelopment.");

});

//Directs the page to the donate page

$('#donate').click(function(){
    //window.location =
'http://facultyprofile.csuohio.edu/csufacultyprofile/detail.cfm?FacultyID=J_F_TURNER';
    //alert("Sorry, this area is still underdevelopment.");

```

```

    var url = $(this).attr('href');
    window.open('/html/donate.html', '_blank');
});

//Directs the page to the reports page

$('#report').click(function(){
    //window.location = '/html/about.html';
    alert("Sorry, this area is still underdevelopment.");
});

//Disables the first header

$("#firstheader").accordion({ collapsible: false, active: false, height:
0 });
});

</script>

<script>
$(function() {
$( "#accordion" ).accordion({ collapsible: true, active: false});
});

</script>

<style>
body{
background-color:728C72; //526E5E; //434A46
}

#headerb{
background-color:#CBD1CE;
width:98%;
margin-left:auto;
margin-right:auto;
//text-align:right;
min-width:960px;
//color:white;
padding-right:10px;
padding-left:10px;
padding-top:5px;
padding-bottom:5px;
font-family:Arial;
border-style:ridge;
box-shadow: -0px 3px 3px 3px #888888;
}

#container1{
background-color:black;

```



```

//width:80%;
width:894px;
height:550px;
margin-left:auto;
margin-right:auto;
//overflow:auto;
border-style:solid;
border-color:white;

}

#holder1{

background-image:url('/html/images/ramindex_splash3.gif');
background-repeat:no-repeat;

position:relative;
background-color:black;
z-index:1;
//float:top;
//margin-top:-260px;
height:100%;
//display:none;
width:894px;
height:550px;
overflow:hidden;
}

#holder2{

background-
image:url('/html/images/mineral_images/Mineral_photos_04_26_10/Edoylerite_micro.JPG');
background-repeat:no-repeat;

position:relative;
background-color:green;
z-index:0;
//float:top;
//margin-top:-600px;
height:100%;
display:none;
}

#headerc1{

position:relative;
z-index:10;
//background-color:F7EDC3;
background-color:white; // #CBD1CE;
//width:80%;
width:880px;
margin-left:auto;
margin-right:auto;
padding-left:10px;
padding-right:10px;
font-family:Arial;
}

#container2{

//background-color:orange;
z-index:6;

```

```

position:relative;
margin-top:-48%;
//margin-bottom:50%;
//overflow:hidden;

}

#accordion{

width:300px;
opacity:0.7;
color:black;
}

#footer{

background-color:white; // #CBD1CE;
//position:relative;
z-index:25;
//width:80%;
width:850px;
margin-left:auto;
margin-right:auto;
padding-left:25px;
padding-right:25px;
padding-top:5px;
padding-bottom:5px;
font-family:Arial;
box-shadow: -0px 5px 8px 2px #888888;

}

#search,#about,#contact,#contributors,#donate, #report, #resources{

cursor:pointer;
//position:absolute;
//margin-left:10px;

}

#holder1 img{position:absolute;z-index:1}
#holder1 img.active{
z-index:3;
width:1000px;
height:600px;
}

#ht{

font-size:150%;
font-family:Arial;

}

#hb1{

//width:300px;
//background-color:red;
font-family:Arial;
}

#hb2{

```

```
//position:relative;
//text-align:right;
float:right;
//width:30px;

}

#hc2{
float:right;
}

#updates, #projects{
cursor:pointer;
}

#f2{
float:right;
}

.beta {
//color;;
}

a {
text-decoration:none;
}

.text {
font-size:80%;
}

#titletext{

color:#375396;
font-family:Calibri;
font-size:90%;
}

#csulink{
text-decoration:none;
color:black;
}

</style>

<body>

<br>
```



```
<h3>About us</h3>
<div>
<p>
<span class="beta" id="ramindexhistory">Ramindex History</span><br><br>

<span class="beta" id="contributors">Contributors</span><br><br>
<span class="beta" id="turnerresearch">Turner Research Group</span>
</p>
</div>

<h3>Contact ACIF</h3>
<div>
<p>
<span class="beta" id="contact">Contact ACIF</span><br><br>
<span class="beta" id="report">Report Problems</span>
</p>

</div>

<h3>Donate Minerals & Spectra</h3>
<div>
<p>
<span class="beta" id="donate">Donate Minerals </span><br><br>
<span class="beta" id="donate">Upload Spectra </span>
</p>

</div>

<h3>Additional Mineral Resources</h3>
<div>
<p>

<a class="beta" href="http://www.mindat.org" target="_blank">mindat.org
</a>
<a class="beta" href="http://www.webmineral.com"
target="_blank">webmineral.com </a>
</p>

</div>

</div>

</div>

</div>

<div id="footer">
<span class="text">&#169; 2013 John F.Turner II. All rights reserved.

<span id="f2"><a id="csulink" href="http://www.csuohio.edu"
target="_blank">Cleveland State University</a></span></span>
</div>

</div>

<br>

</body>
```

## APPENDIX T:

### Euclidean Distance and Mahalanobis Calculation Program "euclidmahalman2.m"

```
clear

%Robert W. Cannon July 21, 2013
%This function is to help calculate the Euclidean distance or
Mahalanobis
%between vectors with average reference vector or a set of reference
%vectors to compare with SIM

%!!Uncomment the section that are needed and comment out the parts not
%needed

%First I need to acquire the reference vector; the vector used here
with
%the the average vector of the all the data

%The sample vector data is stored "sidata_allspecies_norm_comrange.mat"

load vect_lormat_allspecies_norm_comrange.mat;

size(vect_lormat); %Checks the data set dimension

%Optional Unit Vector Calculation
%plot(vect_lormat)
vect_lormatsq=vect_lormat.^2;
%plot(vect_lormatsq)
vect_lormatsqsum=sum(vect_lormatsq);
%plot(vect_lormatsqsum)
length_vectlormat=(vect_lormatsqsum).^0.05;
%plot(length_vectlormat);
vect_lormatnew=vect_lormat';
j=0;
for j=1:1:61
unit_vect_lormat(:,j)=vect_lormat(:,j)./length_vectlormat(:,j);
end
%plot(unit_vect_lormat);

%length_vect_lormat=((sum(vect_lormat.^2)))^0.5

%The avg reference vector is calculated with the mean function; Unit
vector
%can be used also

%avg_data=mean(vect_lormat,2);

%This is the average reference vector

avg_datau=mean(unit_vect_lormat,2);
%size(avg_data)
```

```

plot(avg_datau) %Plot of average reference vector

%These are other refernce vectors; the size must be adjust to match the
%x=(-1:2/1221:1);

%ref_vector=sin(0:10*pi/1221:10*pi);
%ref_vector=(1:1222);
%ref_vector=cos(0:11*pi/1221:11*pi);

%ref_vector=cos(0:2*pi/1221:2*pi).*(x.^4)

%The vector should be appended to the data. The distances needed to be
taken form the calculated matrix.
%The vectors should be organized in to rows for the pdist functions to
%work. Cluster data functions can be used in order to help visualize
the
%data

%appended_vector=[avg_data vect_lormat]
appended_vector=[avg_datau unit_vect_lormat];

%a=appended_vector(:,6)';
%b=appended_vector(:,1)';
%a=[1 1 1 5 6 7 8 9];
%b=[1 2 1 6 5 4 3 2];
%b=[1 1 1 5 6 7 8 9];
%e=[a ;b];
%size(a)
%[c,d]=size(a)

%euclidean_dist=pdist(e)
%sum=0;
%for i=1:1:d
%diff=((a(:,i)-b(:,i)));
%diffsq=diff.^2;
%sum=sum+diffsq;
%end

%eucliddist=sqrt(sum)

%Mahalanobis Single Group

%a vector below is the sample to test
%b vector below is the group average or reference vector

%c=appended_vector(:,4)';

%Average for a single group

```

```
%d=mean(appendd_vector(:,6:10),2)'; %must be the average of the group  
without the sample
```

```
%This section acquires a row from the average and variance matrices to  
be  
%used as a reference
```

```
%test=[1 3 6; 6 7 9; 4 5 7;6 7 9];  
%rtest=[6 7 9];  
%res=ismember(test, rtest, 'rows')  
%index=find(res);  
%[l,m]=size(index);  
%y = test;  
%y(index, :) = [];  
%dnew=y;
```

```
skipflag=0;
```

```
if skipflag==1;
```

```
%Get Average Vector possible sets for each group; will change below
```

```
%avg_vector_set_1=unit_vect_lormat(:,1:4)';  
avg_vector_set_1=unit_vect_lormat(:,:);  
dnew1=mean(avg_vector_set_1); %Remember must be the average of the  
group without the sample; done below
```

```
%avg_vector_set_2=unit_vect_lormat(:,5:10)';  
avg_vector_set_2=unit_vect_lormat(:,:);  
dnew2=mean(avg_vector_set_2);
```

```
%avg_vector_set_3=unit_vect_lormat(:,11:24)';  
avg_vector_set_3=unit_vect_lormat(:,:);  
dnew3=mean(avg_vector_set_3);
```

```
%avg_vector_set_4=unit_vect_lormat(:,25:34)';  
avg_vector_set_4=unit_vect_lormat(:,:);  
dnew4=mean(avg_vector_set_4);
```

```
%avg_vector_set_5=unit_vect_lormat(:,35:40)';  
avg_vector_set_5=unit_vect_lormat(:,:);  
dnew5=mean(avg_vector_set_5);
```

```
%avg_vector_set_6=unit_vect_lormat(:,41:46)';  
avg_vector_set_6=unit_vect_lormat(:,:);  
dnew6=mean(avg_vector_set_6);
```

```
%avg_vector_set_7=unit_vect_lormat(:,47:53)';  
avg_vector_set_7=unit_vect_lormat(:,:);  
dnew7=mean(avg_vector_set_7);
```

```
%avg_vector_set_8=unit_vect_lormat(:,54:61)';  
avg_vector_set_8=unit_vect_lormat(:,:);  
dnew8=mean(avg_vector_set_8);
```



```

%Get the sample vector
[lunitv,wunitv]=size(unit_vect_lormat);

%Calculates new average vectors

for j=1:1:wunitv
    if (j<=5)      %[1,5,11,25,35,41,47,54] Sections of the data for unit
vector matrices
        set=1; %Anatase
        sample=unit_vect_lormat(:,j)';

        %Find and remove the sample from the set
        rtest=sample;
        res=ismember(avg_vector_set_1, rtest, 'rows');
        index=find(res);
        [1,m]=size(index);
        avg_vector_set_1_new = avg_vector_set_1;
        avg_vector_set_1_new(index, :) = [];

        %Calculate the new average vector

        dnew1=mean(avg_vector_set_1_new); %must be the average of the
group without the sample
        %plot(dnew1);

    elseif (j>=5 && j<=11)
        set=2; %Anglesite
        sample=unit_vect_lormat(:,j)';

        %Find and remove the sample from the set
        rtest=sample;
        res=ismember(avg_vector_set_2, rtest, 'rows');
        index=find(res);
        [1,m]=size(index);
        avg_vector_set_2_new = avg_vector_set_2;
        avg_vector_set_2_new(index, :) = [];

        %Calculate the new average vector

        dnew2=mean(avg_vector_set_2_new); %must be the average of the
group without the sample
        %plot(dnew2);
    elseif (j>=11 && j<=25)
        set=3; %Chrysoberyl
        sample=unit_vect_lormat(:,j)';

        %Find and remove the sample from the set
        rtest=sample;
        res=ismember(avg_vector_set_3, rtest, 'rows');
        index=find(res);

```

```

[1,m]=size(index);
avg_vector_set_3_new = avg_vector_set_3;
avg_vector_set_3_new(index, :) = [];

%Calculate the new average vector

dnew3=mean(avg_vector_set_3_new); %must be the average of the
group without the sample
%plot(dnew3);
elseif (j>=25 && j<=35)
set=4; %Diopside
sample=unit_vect_lormat(:,j)';

%Find and remove the sample from the set
rtest=sample;
res=ismember(avg_vector_set_4, rtest, 'rows');
index=find(res);
[1,m]=size(index);
avg_vector_set_4_new = avg_vector_set_4;
avg_vector_set_4_new(index, :) = [];

%Calculate the new average vector

dnew4=mean(avg_vector_set_4_new); %must be the average of the
group without the sample
%plot(dnew4);
elseif (j>=35 && j<=41)
set=5; %Fluorapatite
sample=unit_vect_lormat(:,j)';

%Find and remove the sample from the set
rtest=sample;
res=ismember(avg_vector_set_5, rtest, 'rows');
index=find(res);
[1,m]=size(index);
avg_vector_set_5_new = avg_vector_set_5;
avg_vector_set_5_new(index, :) = [];

%Calculate the new average vector

dnew5=mean(avg_vector_set_5_new); %must be the average of the
group without the sample
%plot(dnew1);
elseif (j>=41 && j<=47)
set=6; %Olivine
sample=unit_vect_lormat(:,j)';

%Find and remove the sample from the set
rtest=sample;
res=ismember(avg_vector_set_6, rtest, 'rows');
index=find(res);

```

```

    [l,m]=size(index);
    avg_vector_set_6_new = avg_vector_set_6;
    avg_vector_set_6_new(index, :) = [];

    %Calculate the new average vector

    dnew6=mean(avg_vector_set_6_new); %must be the average of the
group without the sample
    %plot(dnew6);
elseif (j>=47 && j<=53)
    set=7; %Olivine
    sample=unit_vect_lformat(:,j)';

    %Find and remove the sample from the set
    rtest=sample;
    res=ismember(avg_vector_set_7, rtest, 'rows');
    index=find(res);
    [l,m]=size(index);
    avg_vector_set_7_new = avg_vector_set_7;
    avg_vector_set_7_new(index, :) = [];

    %Calculate the new average vector

    dnew7=mean(avg_vector_set_7_new); %must be the average of the
group without the sample
    %plot(dnew7);
elseif (j>53 )
    set=8; %Sapphire
    sample=unit_vect_lformat(:,j)';

    %Find and remove the sample from the set
    rtest=sample;
    res=ismember(avg_vector_set_8, rtest, 'rows');
    index=find(res);
    [l,m]=size(index);
    avg_vector_set_8_new = avg_vector_set_8;
    avg_vector_set_8_new(index, :) = [];

    %Calculate the new average vector

    dnew8=mean(avg_vector_set_8_new); %must be the average of the
group without the sample
    %plot(dnew6);
end

%Matrix of average vectors

all_avg_vectors=[dnew1;dnew2;dnew3;dnew4;dnew5;dnew6;dnew7;dnew8];

%Mahalanobis Section for multiple reference groups;

```

```

%Attempt to optimize distance results

[rows_aav,col_aav]=size(all_avg_vectors);% Set of all the average
vectors

for k=1:rows_aav;
diffv=sample-all_avg_vectors(k,:);
diffv2=sample'-all_avg_vectors(k,:)';

scatter(sample,all_avg_vectors(k,:)','*')

difftv=diffv';
diffv2=diffv2';

covmv=cov(all_avg_vectors(k,:)'); %good?
covmv2=var(all_avg_vectors(k,:)');

icovmv=inv(covmv);
icovmv2=inv(covmv2);

mdistv(j,k)=diffv*icovmv*difftv;
mdistv2(j,k)=diffv2*icovmv2*diffv2;
end

end

mdistv(j,k)=diffv*icovmv*difftv ;
mdistv2(j,k)=diffv2*icovmv2*diffv2;

clims = [0 7000]; %Adjustable scale for contrast
mahalresults=imagesc(mdistv,clims);

%plot(mahalresults)
%b=appended_vector(:,6);

end
%Mahalanobis results for a single reference vector simulation data only
%There are four calculation methods given below.

%1) First get sample vector

% a=[410];
% a2=[410;420];

%2) Get the reference vector next; here it is the average data vector
% b=[400];
% b2=[400];
%
% mu1=[500];
% mu12=[500; 300];
% mu2=[500];

```

```

%3) Calculate the difference between the sample vector and the average
%vector

% diff=[a(:,1)-mu1 b(:,1)-mu2 ];
% diff2=[a(:,1)-mu12];
% diffv=c-d;
% diffv2=c'-d';

%4) Transpose the difference vector

% difft=diff';
% difft2=diff2';
% difftv=diffv';
% difftv2=diffv2';
% s1=difft*diff;

%5) Get the covariance matrix

% covm=[6291.55737 3754.32851;3754.32851 6280.77066];
% covm2=[6291.55737];
% covmv=cov(appended_vector(:,6:10)'); %good?
% covmv2=var(d);

%6) Get the inverse of the covariance matrix

% icovm=inv(covm);
% icovm2=inv(covm2);
% icovmv=inv(covmv);
% icovmv2=inv(covmv2);

%) Multiply the inverse covariance with the difference vector and the
%transposed difference vector in the corrector order

% mdist=diff*icovm*difft; %for test
% mdist2=difft2*icovm2*diff2;
% mdistv=diffv*icovmv*difftv;
% mdistv2=difftv2*icovmv2*difftv;

%mdist=difft*icovm*diff; %for spectra
% s2=dot(s1,icovm);
%mdist=sum(s2)
% mahal_dist=pdist(e,'mahal')
% [c,d]=size(a)
% sum=0;

%f=cov(a,b)

%for i=1:1:d
%diff=((a(:,i)-b(:,i)));
%diffsq=diff.^2;

%diffsqvar=diffsq.*inv(f);

```

```

%sum=sum+difffsqvar;
%end

%stda=std(a)
%stdb=std(b)
%stda3=3*stda
%stda3=3*stda
%vara=var(a)
%varb=var(b)

%mahaldist=sqrt(sum)

%scatter(a(1,:),b(1,:));

%figure
%hold on
%plot(a,'ro')
%plot(b,'*')

%Mahalanobis results for a single reference vector sample data

%a vector below is the sample to test
%b vector below is the group average or reference vector

appended_vector=[avg_datau unit_vect_lormat];
size(appended_vector);
%1) First get sample vector

%a=[410];
%a2=[410;420];
j=1;
[1,w]=size(unit_vect_lormat);
for j=1:1:w;

c=unit_vect_lormat(:,j)';
d=avg_datau';

%2) Get the reference vector next; here it is the average data vector

%b=[400];
%b2=[400];

%mu1=[500];
%mu12=[500; 300];
%mu2=[500];

%3) Calculate the difference between the sample vector and the average
%vector

%diff=[a(:,1)-mu1 b(:,1)-mu2 ];
%diff2=[a(:,1)-mu12];
diffv=c-d; %must be the difference between all the vectors not the
average!!!!!!

```

```

diffv2=c'-d';

%4) Transpose the difference vector

%difft=diff';
%difft2=diff2';
difftv=diffv';
difftv2=diffv2';
%sl=difft*diff;

%5) Get the covariance matrix

%covm=[6291.55737 3754.32851;3754.32851 6280.77066];
%covm2=[6291.55737];
covmv=cov(unit_vect_lormat(:,:))'; %good?
covmv2=var(d);

%6) Get the inverse of the covariance matrix

%icovm=inv(covm);
%icovm2=inv(covm2);
icovmv=inv(covmv);
icovmv2=inv(covmv2);

%) Multiply the inverse covariance with the difference vector and the
%transposed difference vector in the corrector order

%mdist=diff*icovm*difft %for test
%mdist2=difft2*icovm2*diff2
mdistv=diffv*icovmv*difftv ;
mdistv2=difftv2*icovmv2*difftv;

mahal_results(j,:)=mdistv;
mahal_results2(j,:)=mdistv2;

end
imagesc(mdistv2);
%mdist=difft*icovm*diff; %for spectra
%s2=dot(s1,icovm);
%mdist=sum(s2)
%mahal_dist=pdist(e,'mahal')
%[c,d]=size(a)
%sum=0;

%f=cov(a,b)

%for i=1:1:d
%diff=((a(:,i)-b(:,i)));
%diffsq=diff.^2;

%diffsqvar=diffsq.*inv(f);
%sum=sum+diffsqvar;
%end

```

```
%stda=std(a)
%stdb=std(b)
%stda3=3*stda
%stda3=3*stda
%vara=var(a)
%varb=var(b)

%mahaldist=sqrt(sum)

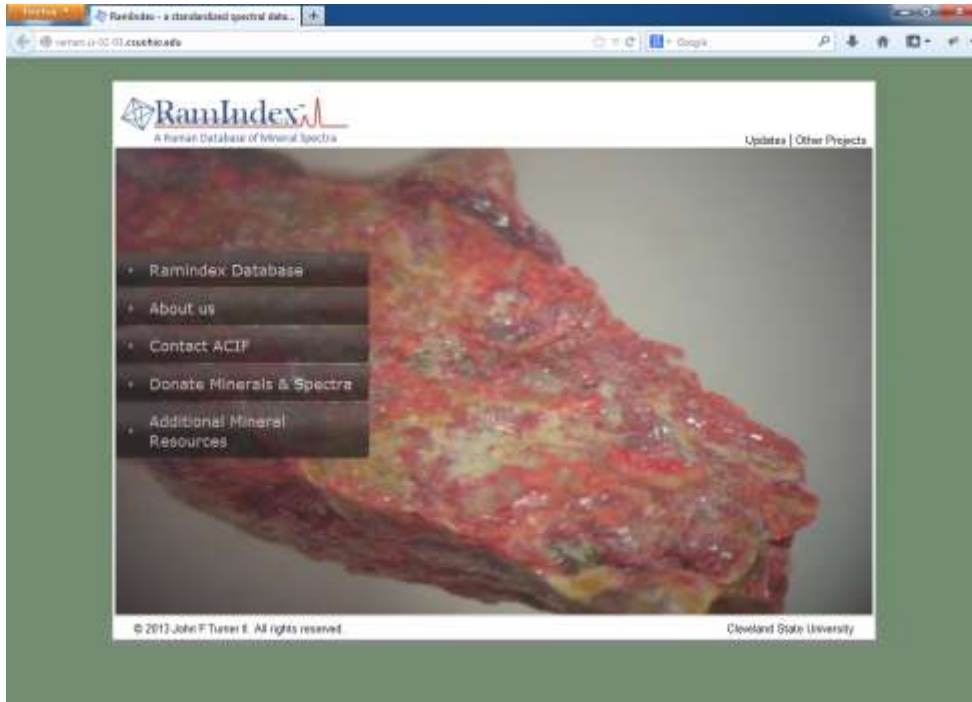
%scatter(a(1,:),b(1,:));

%figure
%hold on
%plot(a,'ro')
%plot(b,'*')
```



## APPENDIX U:

### a) RamIndex Early Screen Shots



### b) Website Index Page

