1 atm pseudo-ternary cotectics

I do this in my spare time so debugging is inadequate. I will send out repairs if needed. **Please report any difficulties**. If I can reproduce a flaw, I can fix it.

Upgrade Notes (more in Readme.txt)

July, 13, 2011 Added a new Legend option, a searate legend diagram

Dec 19, 2010 Fixed the equation for equilibrium crystallization in the Spider Model section, another long-lived flaw! Thanks Jurgen

Nov 12 2010 Fixed an error in converting CaO to ppm. An ancient mistake!, probaly never found because never used! Thanks Sara.

Nov 3 2010 Fixed gross flaw in Pearce, JA (2008) diagram found by Louis R. Bernier.

Oct-Nov 2010 Repaired a round off error in the Histogram plotting logic. This was a tiny fix (from Int to Cint) but a substantial rounding error. Histograms will now be smoother looking. Fixed a flaw in Pearce 2008 diagram.

Aug 31, 2010 further effort to stabilize and make logical the various recalculations of ferric/ferrous ratio.

Aug 11, 2010 Fixed flaw in Sack et al recalculation of ferric/ferrous ratio that caused incorrect plotting on CMAS diagrams sometimes when the ferric/ferrous ratio was reset.

Jan 1, 2010 Extensive effort to make a user friendly version of a REE inversion method devised by Feigenson and Hoffman (see Feigenson et al. 2003 and references therein).

Aug 26, 2009 A series of significant changes. Added more diagrams from IUGS nomenclature and Peacock index. Improved transfer of drawings from Igpet to Word and Powerpoint. Made significant improvement to handling of Isotopic data. Added Hf and Os into AFC modeling. The Model section of Spiderplots now does AFC calcs for Isotopes as well as trace elements.

March 2008 Significant upgrade. Added logic for Hf and Os isotopes. Added AFM calcs for isotopes (Sr, Nd, Hf, Os, Pb) in the spiderplot modeling section. Added Isotope mixing in the Spider Mixing section. Improved screen logic to better handle screens that do not have a 4/3 aspect ratio. Fixed error bars for log plots, bug in Diagram printing, added a few new diagrams

August 2007 Added AFC models to the modeling in the spiderplots

December 2006 Major programming changes that should not affect user. Large change in Folder structure (essentially creating a folder structure)

2005 Improved the Legend and added/repaired many diagrams. Added a text box to calculator. Added a Legend and many smaller improvements and repairs

2004 Major upgrade. Significant change in programming environment, serious attempt to fix international problems involving erroneous truncation of numbers after local decimal characters that are not a "." But are instead a "," Added IUGS classification.

June 2002 Substantial improvements to make Igpet work with Windows XP. Added several more discrimination diagrams and reconfigured several .txt files.

April 2001 Repaired CoDoPo option in Spider modeling. Added a few more .txt files.

March 2000 Igpet uses windows metafiles (.WMF) to transfer graphics to the clipboard and store them on a disk. Earlier Igpet versions relied on a background page to keep aspect ratios in place. This backpage is now an option

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Graphical Interpretation of Geochemical-Petrological Data

Igpet and Mixing can display data beautifully and make a surprising variety of complicated calculations, but rarely do these tools prove anything! What these programs can most easily and reliably do is prove hypotheses incorrect. Usually, one can conclude that a hypothesis, such as fractional crystallization, is consistent with available evidence, not that it is proved. All too often this inherent limitation is forgotten and weak hypotheses are deemed proved on flimsy graphical evidence. In my experience the worst pitfall of this software is the ease with which fuzzy thinking is translated into attractive diagrams that are pasted into papers and theses without much useful thought. I am intimately familiar with some varieties of misbegotten interpretations because I have done them myself! The paragraphs below summarize some of the false paths Igpet can lead a student down.

The correct approach to solving the problem of how a suite of samples of igneous rocks might be related to each other is first to look at the hand samples and thin sections of all (or at least half!) of the samples. The thin sections can immediately set the tone for the problem at hand. Assuming the samples are all from the same volcano or from a group of geographically and temporally associated vents, one can start wondering about how they are related. My preferred sample set is a long stratigraphic sequence from a caldera wall. Nature is rarely so co-operative. If the samples are aphyric, or nearly so, there is a reasonable chance you may be examining a set of separate melts, so some type of partial melting hypothesis can be considered. If a plot of MgO versus K_2O is a mess, with a large K_2O range and little or no consistent potash increase as MgO decreases, then you should get more incompatible element data, especially REE data, in order to test various partial melting models. If, instead, there is a strong inverse relationship between potash and magnesia, then fractional crystallization becomes the hypothesis of choice.

The presence of abundant phenocrysts and, especially, the presence of disequilibrium textures and assemblages should make one worry about mixing and accumulation processes. If olivines and quartz are in the same thin section, then something is wrong! Either mixing or assimilation is being signaled except in the rare cases of some Fe rich granophyres with fayalite and quartz. Electron microprobe analyses of minerals (olivines, plagioclase, clinopyroxene, etc) that define two distinct populations (a bimodal distribution) are fairly definitive evidence for magma mixing that has occurred too recently for the phenocryst evidence to be swept away by the thermodynamic drive toward equilibrium.

Igpet is a tool but not a textbook. There are several useful petrology and geochemistry books. The more elegant calculations in Igpet either came from Albarede's 1995 book, Introduction to Geochemical Modeling, or are reproduced there. The reference list at the end of this manual is included to be **USED**, especially, some rather old references: e,g. O'Hara (1968 and 1976) for CMAS projections; Bryan, Finger and Chayes (1968) for petrologic mixing calculations; Chayes (1964) on the shortcomings of Harker or Fenner diagrams; Pearce (1968) for clever methods to test fractionation hypotheses using major elements (more recent refs discount the use of Pearce diagrams- see Rollinson (1993) for a summary.; Langmuir et al, (1977) for the mixing equation;

DePaolo (1981) for AFC calculations.

Another area where Igpet graphics must be complemented by careful reading is the use of the many pre-designed diagrams (e.g. for CMAS projections, rock nomenclature and tectonic discrimination). Many of these diagrams have specific limitations on their use. Igpet points out the rudiments of restrictions using the nota bene (NB) line at the top of many diagrams. However, there is no substitute for reading the original reference. Rollinson has done a terrific job in comparing and summarizing many discrimination diagrams in his 1993 book, <u>Using geochemical data: Evaluation, presentation, interpretation.</u>

One of the dirty tricks in Igpet is the automatic setting of the range of X and Y axes. The automatic setting is useful as a starting point but it is **DUMB**. Your rock suite may be very homogenous but Igpet is dumb and will stretch the X and Y range to the full amount possible. In such a case, the variation that appears (a random mess) is just noise. Don't panic that your data are of poor quality, just look at the range and adjust it.

Be wary of log-log plots. I almost regret including the Log_{10} function in Igpet. I am coauthor on papers that use log-log plots. The excuse for using log transformation is the huge range in source compositions for arc rocks; depleted mantle at one end and hydrous fluids highly enriched in incompatible elements at the other. It is satisfying to see the full range of the mixing line between the end-member compositions, but all the detail concerning the relationships between the actual samples becomes highly compressed. It is a common mistake in science to propose spurious functional relationships based on roughly linear data arrays in log-log space.

Be wary of "trends" or "trend lines." I do not think that these terms have any actual meaning. Igpet calculates statistics needed for linear regression, including the Pearson correlation coefficient, r, and the Spearman rank order correlation coefficient, r'. You will need a competent statistics text to understand these parameters. I hope you have had a good course in applied statistics for the physical sciences. I was unlucky and suffered through a horrible course on statistics for economics and have a weak statistical background as a result. If you hear about a good stats course, take it.

Know your data and use the multitude of symbols judiciously. Few of the volcanoes I have looked at are homogenous. Identifying subsets, defined stratigraphically or geochemically, almost always leads to increased understanding. Even among basalts from the same volcano, there are usually apples and oranges. Using the same symbol for two different magma types results in a hodgepodge that cannot be interpreted in detail. Igpet now has 36 symbols, more than enough (for most but not all) to define subsets of any reasonably sized sample suite. The drive to subdivide and pigeonhole can be overdone and I doubt there are any hard and fast rules. I tend to overdo it and then back off and combine similar groups. At the other extreme, some geochemists never subdivide at all.

Obviously, I have turned into an opinionated grump in my advanced age. However, on the

brighter side, I hope you will have serendipity with Igpet. Several times Igpet has allowed my students and me to discover unsuspected order in volcanic geochemistry. The ease allowed by Igpet allows lots of experimentation. Sometimes there will be too much and you will end a session of data examination lost, dazed and confused. Get some sleep, then try again and try to stay focused on what is plausible.

The following argument, derived from Patino et at. (2000), describes an approach to looking at data. The problem was a new batch of ICP-MS data for Central American volcanic rocks and for the sediments just about to be subducted beneath Central America. In some plots of pairs of incompatible element ratios, like Ba/La versus La/Yb, there were clear systematics indicating mixing and melting relationships between the most plausible sources; the mantle and the sediments being subducted. However, most possible ratio-ratio plots of incompatible elements produced just a mess, not systematics. So why do some plots work and others fail? One problem was the complexity of the source. Most of the source was MORB-like mantle but the subducted plate contributed a basalt layer and two sediment layers, providing a minimum four sources. Plausible processes, such as partial melting or hydrothermal transport added further complications.

The first criterion we used to select useful trace element ratios was to identify the incompatible elements with the largest difference between the two sedimentary units. Arranging the elements in order of their overall hemipelagic/carbonate ratio (U, Cs, Th, K, Pb, La, Y, Ba, Sr), we saw maximum difference by comparing element ratios from opposite sides of this spectrum (e.g., Ba/Th and U/La). On the other hand, we could minimize the confusing effect of having two sediments by looking at elements near each other on the spectrum (e.g. Ba/La or U/Th).

I should mention why we ignored Sr, Y and Cs. With Sr there is the reality of compatibility with plagioclase, so even moderate degrees of plagioclase crystallization cause departure from incompatible behavior. In log plots such as spider-diagrams, this is generally not a problem because the loss of Sr to plagioclase is not great. However, in linear plots (e.g. element vs element or ratio vs ratio) the loss of Sr to crystallization becomes a large effect. Like the HREE, Y is only moderately incompatible and certainly less incompatible than the others. In the case of Cs, weathering is our excuse for being suspicious. Central America is hot and wet and Cs movement is one of the first signs of leaching, even in very fresh appearing rocks. This can be a very large effect and visible even in spider-diagrams.

We found that the useful ratios, the ones with apparent systematics, were defined by separation. That is, plots where the potential sources (mantle wedge, subducted MORB, carbonate sediments and hemipelagic sediments) occupy separate fields in ratio/ratio plots. The mantle wedge and MORB components often overlap in the ratios of highly incompatible elements. Therefore, we preferentially selected pairs of ratios where MORB + mantle, carbonate sediment and hemipelagic sediment defined a triangle. Where two components are close to each other, as the two sediments are in Ba/La versus U/Th, the field of volcanic data collapsed into an apparent binary mixing array between mantle and bulk sediment.

In general, even with a trimmed ICPMS data set (Cs, K, Rb, U, Th, Nb, Ta, La, Gd, Yb, Zr, Hf, Pb, Sr, Ti) you can plot a huge number of combinations. The reduced list above can be further trimmed of Hf and Ta, which behave like Zr and Nb, but even so you have 13 elements from which to pick 4. I think that provides 715 possible ratio-ratio plots, most of which are useless. What you are doing is looking at 13 dimensions of space and trying to discover volumes that have clear systematics. This happens when some components line up and fold into each other simplifying the problem.

If you have 4 or 5 sources, you have trouble because ratio-ratio plots become very confused if there are more that 3 well separated sources. The place to start is to look at the plausible sources. Do any sources overlap on nearly all elements, allowing the problem to be simplified? The next step is to find at least a few ratios that are nearly the same for two or more otherwise distinct sources. This allows a simplified window, folding a couple of sources together. Finally, focus on plots that show the largest separations among source components. Having large separation is crudely like being perpendicular in the mathematical sense. So you are seeking windows within the data space where the sources are either parallel (folded into each other) or perpendicular. In these views, the systematics will be the most clear. Many other plots may be similar but suffer from being less orthogonal and have confused and unconvincing data arrays. The plan is to find the clearest views and then model them.

Another approach, of course, is to read the literature and do what other people do and try to understand and apply their approach. I like to read literature with my computer on (actually it has to be on these days because I read mostly pdf files). So I have a journal window open and I open Igpet and try to duplicate interesting plots with my favorite data (Central America and many subsets). I highly recommend this. It is remarkable how different arc geochemistry can be given the similarity of process. To me, each convergent margins simply has different open widows, depending on source differences and process variations.

Installing Igpet

Igpet is a 32-bit program so it should go into the Program Files (x86) folder on modern windows machines. A setup program, called something like, **SetupIgpet2011.exe**, installs Igpet. All of Igpet's control files and all the data files shipped with Igpet will be copied to a directory, normally called Igpet2011 or whatever the current year is. Put this folder in Program Files (x86). I sometimes use My Documents instead but this may now always work in Windows 7. Several subfolders within Igpet2011 are created for different file types.

Tutorial

The best way to learn Igpet is to use it on one of the data files shipped with it. The next few pages leads you through the major features available in Histograms, XY plots, Tri plots and Spider diagrams. Along the way, most of the functionality in Igpet is demonstrated. So, from the Windows Start Menu select: Igpet. The main Igpet window appears. Options can be selected by clicking menu items or buttons.

Read a File

First, click menu **File**, **Open File**, then use the file dialog box to select a data file with an extension like .TXT, .ROC, .MIN. For this tour select FUSAMA.TXT from the folder, called Data Files." After the data are read the **Plot** menu is activated.

Make a Histogram

Click menu **Plot, Histogram** and you will be asked to select the X-axis variable for a histogram using the Variable Menu, which is a grid of buttons that includes a primitive calculator. There is a text box below for entering formulae.

Calculator
Igpet's calculator consists of a row of operations and a row of buffers that store the results of the operations. You can convert from oxides to ppm, normalize an element to its mantle source value (S-norm), etc. You can add, subtract, multiply, or divide. When you make an operation, the result is stored in one of the buffers, and the new name is listed in the row of buffer buttons. Quite complex equations can be put together and their names may get too long to be completely listed in the available space. This is not a problem as long as you remember what you are doing. When you run out of buffers, the program goes back to and overwrites the first buffer.

Text Box Equation Parser
A text box, below the calculator, allows you to directly enter simple equations, bypassing the calculator. The recursion routine doing the work seems robust, but be wary. If you get something unusual you should replicate it with the calculator.

The **Histogram** function plots bins using the color of the symbol for each analysis. To make a more pleasing looking histogram you can select **Symbols** from the **Edit Menu** and click the **One symbol for all** button. Draw a normal curve on the histogram using the **Distrib** button. This function uses the mean, std. dev., N and bin definition to scale the normal curve. Statisticians recommend beginning any examination of data by first looking at univariate statistics. Try a few plots like SiO_2 or Na_2O+K_2O or CaO/Al_2O_3.

Make an XY plot

Click the menus **Plot, XY** and you will be asked to select the X-axis variable. Select X, and then select Y in the same way. A graph will now appear on the screen. Buttons above the graph allows you to change the diagram and make some petrologic calculations. A plot of SiO_2 vs. K_2O is useful to show the uses of these buttons, so if you have plotted something else, click on **New X** or **New Y** to create a SiO_2 vs. K_2O plot.

Error Bars
If a single variable is selected via the buttons (e.g. SIO_2 or TiO_2 etc) and if the data column for the variable is followed by a column beginning with "error", then Igpet recognizes the error field as plus/minus error and plots an error bar. Use Boqueron.txt as a test and plots SiO_2 versus TiO_2. Error propagation will eventually be added but for now error bars work only for single columns. You can calculate propagated errors in Excel. For example, have Ba/La as one column and its propagated error as the next.

Identify a particular data point
The FUSAMA file includes analyses from a high-alumina volcano (Fuego in Guatemala), a calc-alkaline volcano (Santa Ana in El Salvador) and a tholeiitic volcano (Masaya in Nicaragua). You can determine which symbols stand for which volcano by clicking **ID ON**. The identify function starts by causing the first sample to be highlighted on the screen. The sample name is shown just to the right of the top line of buttons. Now move the mouse to any data point and click. This sample will be highlighted and its name will be written. Use the newly activated buttons, **Next** and **Prev,** to move forward and back through the data, highlighting successive data points. To pick one sample from a list, click on **Pick**. A column of sample names will appear. Double-click SA206. This is the most mafic sample from Santa Ana and it should now be flashing. The **Name** button will give you a quick look at where all the samples plot.

The identify buttons allow you to get to know your data. Furthermore, they are essential for selecting endpoints for the Mix and Model options.

Add a Legend
The **Legend** button asks you to select a legend file. There is a legend file for the Fusama data, called: FusamaLegend.txt. Use this file as a model for creating custom legend files for your own

data. These files are tab delimited text files that are easily made with Excel. The first column is an integer, a key to a symbol, the second column is a name or description.

Fine-tune the X and Y axes

Igpet automatically scales the X and Y axes based on the spread of data. This is convenient for quick looks, but ***it can be very misleading,*** especially if one or both axes has a small range of variation. Here, the computer can make you imagine variation, when, in fact, the spread is noise.

To change the axes, click the **Axes** button near the top of the main window. You get a list of parameters you can edit. Most are self-explanatory but the choice of the interval to draw long ticks may take some practice. If you want just small ticks enter 0. The most commonly used values for long ticks are 2, 5 and 10. Just experiment and find out what you like.

Switch the X and Y axes

The button **XY-YX** allows you to instantly switch the axes.

Change aspect ratio or position of a graph

Aspect Ratio in the **Edit Menu** allows you to change the shape of your graph and to change the position it will occupy on a printed page. The default aspect ratio for Igpet is a rectangle, suitable for 35mm slides. In many instances it is better to use a square or box. A final option allows you to customize the shape (within limits) to suit your purpose.

The **Position** of the graph can be selected from a list of options in the **Edit Menu, Position**. These positions are specified in a file called Page.dia. Using Notepad, you can modify them to suit your needs. See Appendix A for details.

View a third dimension

Write Values in the **Edit Menu** lets you display on the current plot the value of any parameter available through the calculator. For example, on the SiO_2 vs. K_2O plot, you can write the TiO_2 values of each sample. Click **Write Values** again to remove the numbers.

Select subgroups with symbols

Because there are three volcanoes in FUSAMA, a linear regression would have little meaning. The easy way to eliminate two of the volcanoes is to click **Symbols** in the **Edit Menu**.

Click **Refresh** to see the symbols or just click in the tall window. A symbol is eliminated by clicking on the adjacent check box. To select just the Santa Ana data, note the position of the red circles. Click **Deselect**, then click the check boxes adjacent to open red circles. Now only Santa Ana data will be plotted.

The **c** buttons in the line and fill columns allow you to change the color of symbols or lines using the Windows color dialog. You can explore more pleasing combinations and save the RGB definitions of the colors in a file, like mysyms.sym, if you wish to make a new symbol file.

Take a minute to examine other options in the Symbols window.

Basis for Symbols allows four choices for controlling symbols, **Jcode, Kcode, Lcode** and **Scale to Variable**. The first three are parameter names in data files that Igpet recognizes as potential symbol codes. Having three symbol parameters is probably overkill, but you may find it useful to subdivide your samples into different subsets on totally independent criteria, such as stratigraphic grouping; petrographic characteristics; TiO_2 concentration, shape of REE pattern, etc. The **Scale to Variable** button allows a plot to be "contoured" by plotting different symbols for different ranges of a parameter. For MORBs, a plot of water depth versus Na_2O, contoured in MgO, is a useful way to look at this correlation, proposed by Klein and Langmuir (1987). This is analogous to the **Value** button described above.

New Size allows you to modify the sizes of the symbols, shrinking or enlarging them all. This is a useful fine adjustment when you are making a publication quality diagram.

Black syms allows you to remove the effects of a black and white printer's effort to reproduce color by drawing dithered shades of gray. Now that journals are publishing colored diagrams this option is less necessary. **Dflt sym col** reverses the effect of **Black syms.** You can use the file, grey.sym, to get greyscale symbols. In the **Symbols** page click **New sym file**.

Tie Lines draws tie lines between each successive datum, which is nice if the data are in some kind of order (e.g. stratigraphic height). but creates a mess in most circumstances.

1 sym for all allow you to pick one symbol that will be used for all the points.

The **Font Style** button brings up the font dialog box. It is best to stick with True Type fonts. These have the best chance of staying the same and looking good on all output devices. The default Font Size is a little large for highly populated spiderdiagrams, so use this to make the X-axis labels smaller and non-overlapping.

Three edit fields for line widths allow you to control how fat the lines are in Igpet. The useful range is from 1 to 15 or 20. The colored margins of symbols may be invisible on black and white printers. If so, use **Black Syms** and the symbol borders will reappear.

Four buttons control background colors. The screen and all output devices have two colored areas, one for the page and one for the XY box or TRI polygon. The advent of color printers created a desire to print in vibrant color. Furthermore, one can transfer colored diagrams to graphics programs, like CorelDraw, and have slides made directly from CorelDraw pages. **Pagecolor** and **Boxcolor** let you set these two areas to any possible color. **Whitepage** and **Defaultcolor** do what their names imply.

The edit fields, **pg width** and **pg length** control the logical page size. Regardless of whether you finally send output as Portrait or Landscape images, the width and lengths here are always the dimensions for Portrait mode. This control may help you pass graphics more perfectly to different draw programs. The reason it is included is that Micrographxs Draw, CorelDraw's clipboard-paste and CorelDraw's WMF-import all appear to use slightly different default page sizes.

Now click **OK** and return to the main screen.

Select Subsets of your data
The **Select Subsets** option in the **Edit Menu** allows you to filter your data through several possible limits, matches and exclusions. For example, some of the high silica samples of Santa Ana are from domes at the adjacent Coatepeque caldera. Including them in a linear regression might be a mistake, to eliminate them, click on **Select Subsets** and then doubleclick **SiO2** in the leftmost panel. The next panel fills with a list of SiO2 values. Above the third panel set a Minimum of 0 and a Maximum of 58. Now click **Add to limits** and then **Done**. A graph without the high silica points will now appear. There are many ways to limit, match or exclude data. With very large datasets that include several different units this is a nice way to look at the whole data file and then just a few subsets, such as individual volcanoes.

Linear regression calculation
Click on the **Regress button** to draw a linear regression line. The line can be drawn through either the range of X-values or the length of the X-axis. After the line is plotted, the slope, intercept, R^2, r, r', n, t and F appear in a window. The slope and intercept and their errors (+- 1 SD) are in scientific format (thus 1.16E-01 = 0.116). After making any needed notes on the regression parameters, click **OK** to go on.

Regression parameters (slope, slope error, intercept, intercept error) can be printed on the diagram or saved to a text file, called stats.txt, or to a file for the CoDoPo inverse modeling procedure, a *.ig file. Next, you are asked to add the line to the plot or not.

Sometimes you may want to plot all the data, but calculate a regression on just a subset. If the data to be excluded have a different symbol, you can use the **Symbols** option to temporarily exclude the unwanted data. You can use the **Select Subsets** window in similar fashion.

Notes above the diagrams
As mentioned above, regression results can be printed above the diagram. Before copying the plot to Word or PowerPoint you can remove the extra notes using the **NB off** toggle button.

Hyperbolic mixing
The **Mix-Two Endpoints** button uses the equations derived by Langmuir et al. (1977). It works for isotopic ratios (Sr, Nd, Pb), oxides or elements, oxide or element ratios and the ppm, source normalization and Log options on the calculator. It will not work for complex equations.

First, you need to use the identify buttons (**ID ON**) to choose which samples to use as endpoints. Once you have selected endpoints, click **Mix**.

Second, select the first and second endpoints using double-clicks.

Third, pick one of four options for plotting tick marks on the mixing curve. Except for option N (none) six ticks will be plotted. The values for the options in % are:

E	0	20	40	60	80	100
S	0	0.5	1	3	12	60
T	0	0.1	0.2	0.3	0.4	0.5

Finally, you can limit the hyperbola to between the endpoints or allow it to span the X-axis. For a simple linear plot, like SiO_2 vs. K_2O, the hyperbola becomes a straight line. I'm not sure there are any interesting mixing plots for FUSAMA but there are in the file CENTAM.ROC. These data will allow you to reproduce the diagrams in Carr et al., (1990).

The **Mix-Least Squares** button fits a hyperbola to all the data visible on the screen. This will produce a mess unless you have a well defined curve. It is best to use this on a plot like a/b vs. c/d. Because it is quite a fussy equation to fit, a success is a strong positive indicator of mixing, providing, of course, that field data, thin section observations and basic geochemical patterns indicate mixing. A failure here suggests that a mixing case may have imprecise data or that AFC is operating, so the case is not simple.

Model

Model allows you to calculate paths for fractional or equilibrium crystallization or the AFC (assimilation-fractional crystallization) process. To examine the AFC capabilities properly, you should get DePaolo (1981) and read the file DEPAOLO.ROC. This file will allow you to reproduce Figure 3 in DePaolo's article and, in the process, learn how this modeling works.

For the Santa Ana graph of SiO_2 vs. K_2O, use **ID ON** to locate a "parent" on the lower left side of the data array. Now click **Model**. Select FC for fractional crystallization. Then select the "parent" (Co) and the model parameters. Bulk distribution coefficients of 0.7 for SiO_2 and 0.01 for K_2O are good starting points. You can make several models and make a real mess of the graph if you save all your models. To clean it up, click **Aspect**, then **Quit**. A pad of paper is useful to remember what models are worth including in a final plot. Overall, this option is a useful first pass, qualitative way to develop a FC, EC or AFC model. To do this properly you need to consider all pertinent elements at once and include realistic modal and partition coefficient data. This is done in the model option available with spider diagrams.

Make a Triangular Plot

Triangular plots are created from the **Plot Menu** with the same calculator used for XY plots. To make a triangular plot, click **Plot TRI**. You will be asked to define the three end members, X, Y,

Z, (e.g. Na_2O+K_2O, $Feo+.8998*Fe_2O_3$, MgO). (Note: 0.8998 can be inserted in a buffer by pressing C for "constant")

A new button appears, **Quad**, which allows you to cut off one or more corners of the triangle. Cut the top by specifying 0, .5 when asked for the Min, Max of the Top Apex. This will give a quadrilateral. Cutting the extent of the triangle may allow it to be drawn at a larger size and Igpet will do so automatically.

Make a Spider plot

Spider diagrams are great way to see large variations in incompatible elements at a glance. Because of the log scale you cannot see the detail seen in XY plots, especially plots of incompatible element ratios. Nevertheless, it is a powerful tool. Unfortunately, it is also a source of Babel because there are new spider diagrams almost in each issue of a geochemical journal. The best spider diagram will eventually win out (I hope). The best, according to reviewers of my work, is primitive mantle normalized. The one by Sun and McDonough (1989) is a good one and there is a revised version from 1995. I now use these two almost exclusively, except, of course, for REEs. The general idea of a spider plot is best expressed in the "classic," the REE plot. The most incompatible element is on the left, the least incompatible element is on the right. The spacing between elements would ideally be related to degree of incompatibility but most diagrams use an ordinal scale to make life easy for draftsmen and computer programmers. For REEs this leads to blank spaces for elements not determined in particular instruments. In Igpet the missing elements show up on the x-axis but no symbol appears (e.g. Pm and, often, Tb).

Repick, **NewSpi** and **Y-Scale** are special buttons for the spider diagrams. To see them, first select **File-Open File** Centam.txt. Now, select **Spider** from the **Plot** menu. From the list of choices that appears try REEs first, by double-clicking on the top entry. Next select a few samples to plot from the list that appears by double-clicking GUM4 and GUT102, from Moyuta and Tecuamburro volcanoes in Guatemala. Use **Repick** to select different samples, **NewSpi** to pick a different spider diagram, or **Y-Scale** to fine-tune the Y-axis. **Nrm/Samp** allows you to switch to one of your samples as the normalizing standard. That sample plots horizontally at 1.

Modeling and Mixing in Spider plot*s*
Elaborate partial melting and crystallization models can be performed when a spider diagram is plotted. This requires partition coefficient files (*.pc.txt), a starting composition, and knowledge of melting models. The book by Francis Albarede, Introduction to Geochemical Modeling, should be read carefully before using these modeling tools. To see examples of how this powerful set of options can be used, see Feigenson et al. (1996) or Patino et al. (2000). The CoDoPo option in spider modeling uses a trace element inversion method developed by Feigenson and Hoffman and used in Feigenson et al. (1996, 2003). The AFC trace element models of DePaolo (1981) use a parameter r, the ratio of assimilation rate/crystallization rate.

For the three cases r<1, r=1 and r>1, different ranges of F are suggested by Igpet. Study the DePaolo paper to understand what is going on, rather than blindly using the software.

Explore the **Mix** option by clicking the button. You can select up to 5 samples that can be mixed using integer weights, decimal fractions or %s. Thus, 3,1 and .75, .25 and 75, 25 produce the same result when mixing two samples. You can average 5 samples by selecting them and giving each a weight of 1. More interesting would be modeling a specific mantle by mixing components, for example, by adding 95 DMM and 5 HIMU, etc, etc. You can bail out of the Mix function using the **Quit** button.

The **Model** option models melting and assimilation/crystallization processes. You start by selecting a model, e.g. Aggregated Fractional Melt, then you select whether melting is modal or non-modal (Pi's<> Di's). You pick a partition coefficient file (a pcs file), a mantle mode, a melt mode (if non modal melting), and a set of % melts. The melt mode for the P values includes a manual option and a set of three possible high pressure norms, Spinel Lherzolite, Tshermaks mode and Garnet Lherzolite. The 'rules' for calculating these three norms are in Figure 3 of Keleman et al. (1992).

You can run the melt equation forward (the default) or backward (inverse) by toggling radio buttons. When all is set, click the **Make Calculations** button, the bulk D's will appear, then the P's in non-modal melting, then the models will be plotted on the spider diagram as black crosses. Unlike the simple models in the XY plot, these data are now added to the data in memory, so you can go on to make XY plots, especially ratio versus ratio diagrams, to look in detail at your models. To save any models permanently, you must go to **File-File Operations** menu and **Save** the file. Usually, it is best to save the file using a new name.

Output Options

Before printing or saving a diagram, explore the **Edit** menu options. For printing, the colored backgrounds can waste a lot of ink on drafts, so two options in the **Edit** menu allow one to switch back and forth between colored (**color)** and white (**white**) rectangles. If you don't like colors at all, you can set the defaults to white (255,255,255) in your favorite sym file. Change boxcolor and pagecolor, located near the end of the file. Use the Windows Notepad accessory. See section below on *.sym files.

You can change the orientation of the y-axis label using two options in the **Edit Menu**. The reason for this is that vertical fonts to not pass unscathed through the Clipboard or a Windows metafile (WMF) and then onward to a document. CorelDraw almost translates them properly, but Micrographxs draw programs and Microsoft Word do not allow them. To pass diagrams to a graphics program or word processor, it is best to send them as horizontal fonts and rotate them after you get them there, so Igpet does this automatically. The default orientation of Y axis labels can be set in the **Preferences** menu. The vertical choice is valid only for the Screen and Printer.

Print

The **Print** option in the **File Menu** sends output to the printer. You first are asked if this is the last plot on a page. This query allows you to place several diagrams on a page rather than printing just one. Just keep track of what you are doing! The printer dialog box will not appear until you click **Yes**.

If your first plot, using a vertical Y-axis label, comes out reversed or odd, then you need to change the **Printer's Y-axis** setting in the **Preferences** menu. The default, as shipped, is 90º which works for HP LaserJets in normal configuration. HP inkjet printers prefer the more logical value of 270º. Make changes in the **Preferences** window and be sure to save the new preferences!

To the **Clipboard** from the **Edit Menu**

The clipboard is the best way to transfer a diagram to a document. To use it, make sure both Igpet and the program you plan to copy to are both running. The **Copy to clipboard** option in the **Edit menu** lets you choose between **Diagram** and **Diagram and background page**. The first option is best for Powerpoint and fine for Word, as long as you don't need to edit the drawing. **Diagram and background page** is more stable if you want to edit the diagram in Word. The **Diagram** option is the simplest and it is always best for Powerpoint. After you paste a diagram into Word, use the Format-Picture-Layout-Tight (or Square) to allow flexible placement of the picture.

The drawings that fail during editing in Word contain large data sets. Be wary of distortions when you try to edit a data-rich drawing copied from Igpet into Word. First, right-click on the drawing and then select Format-Picture-Layout. I use Tight or Square, depending on my mood. Now, click the expand arrow in the Draw toolbar located at the lower bottom of the Word window (use View-Toolbars if it is not there) and Ungroup the drawing. You will be asked if you want to convert from a picture to a Microsoft drawing object. Click yes and see if the drawing gets screwed up. The fonts should increase slightly but otherwise nothing should happen. If you have many data and distortion occurs, go to Powerpoint and make your edits there. Alternatively, use Edit-Copy to clipboard-**Diagram and background page**. Then paste the diagram and select the Format-Picture-Layout-Tight followed by Draw-Ungroup (multiple ungroupings may be needed). Once everything is ungrouped, edit at will.

In Powerpoint you can usually just right-click on the drawing and select edit picture. Right-click again and select groupings. Ungroup and then keep ungrouping until everything is ungrouped. Go to the Draw toolbar at the lower left, and try ungrouping there as well. After everything is ungrouped, you can remove the background and edit. To make the drawing larger, click Edit-Select All and then Draw-Group. Now use Format-Object and be sure to maintain the same horizontal and vertical scales. A setting of 167% will expand the diagram to the full Powerpoint slide size. When you are finished editing and sizing, copy the group from Powerpoint to Word.

To see your diagram on the clipboard, activate the Windows Clipboard Viewer. You can just paste a diagram into Adobe Illustrator. AI seems to slightly screw-up the colors and squeezes the letters and numbers. Clipboard graphics cannot be modified in Micrographxs Designer.

Save Diagram to wmf file from **File Menu**
Windows metafiles are lists of Graphics Device Interface (GDI) calls that create a vector graphic. You can save a diagram for later import into a draw program or word processor by clicking this menu option. First, choose between **Diagram** and **Diagram and background** page as in the copy to clipboard option. A file dialog box will open. Keep the .wmf extension because that identifies the file type. Microsoft Word and PowerPoint, CorelDraw and Micrographx's Draw and Designer treat these files differently, but will import *.wmf files. The size of a diagram is preserved but the placement on the page may not. Put one diagram in each *.wmf.

Preferences

The **Preferences** menu brings up a window that allows you to customize Igpet. Three buttons allow you to specify the path to the directory where you keep your data files, the file used for symbols and the file used to read the normalization factors for the S-norm function in the Calculator. Radio buttons allow you to select three other options. The first is a file filter that allows you to set limits on the data that will be read from a large data file. The other two allow the y-axis labels to survive printing and transfer to graphics programs. The orientation of the Y-Label should be Horizontal for transferring graphs to graphics programs or word processors. The Printer's Y-axis can be toggled to fix garbled vertical y-axis labels on your printer; rather than adjust your printer, adjust this setting in Igpet.

Near the upper left of the preferences window is a box. It is advantageous to scale the size of Igpet to a decimal fraction of your screen, this allows Igpet to be a moveable window, rather than filling the whole screen. In 800 by 600 mode I commonly use 0.95 to allow the task bar to stay visible. Put in a number less than 1 (e.g. 0.90).

The changes you make in preferences will not do much unless you save them. Your choices go into igpref.ini for use the next time you start Igpet. The radio buttons and any changes to the Misc area take immediate effect (but not lasting-unless saved) but other changes do not.

Data Handling in the File Menu

Options for Additional Parameters
Igpet can calculate and store in RAM a large number of parameters derived from the major and trace element values. The derived parameters can be saved to a file, but this is not usually worthwhile, because it is slower to read such data, than it is to calculate it. If you want to transfer some of these parameters to a spreadsheet, then it may be worthwhile. Before adding derived parameters make sure the data matrix has enough room.

Reset Matrix Size (File Menu)
If you plan to add optional data fields, you should check the current size of the data matrix before you read your data file. Click this menu item to see default matrix size. The first number (rows) tells you the maximum number of analyses. The second number (columns) tells you how many fields are allowed. You start with the number of fields in your data file. Then add the following:

CIPW	26
Pearce	17 or more
Extra	7 or more
Normalize	1

Putting all this stuff into the data matrix means adding about 50 fields. It makes the calculator difficult to use and is usually not necessary. The best plan is spend a session working with the CIPW Norm, then re-read your data file and work with the other parameters.

The single data field added by the Normalize routine will be unloaded if nothing else has subsequently been loaded. The other parameters can't be unloaded, to get rid of them, you have to re-read your data file.

Norm to 100% (File Menu: normalize to 100%, water free, Fe as FeO)
If there is a limited range of silica values (e.g. 49-55) in a suite, scalar effects will appear large. The largest analytical error is usually silica, just because it is more than half of most rocks. Other scalar errors occur if the rock is altered (added water, oxidation of FeO, etc.). Furthermore, most analyses are subject to minor systematic or gravimetric errors leading to values that are slightly high or low. If errors like these occur then silica will be visibly affected, whereas K_2O or other oxides will appear unchanged. This is the general rationale for using this subroutine. These effects are part of the closure problem (Chayes, 1964). This routine finds oxides of 13 elements: Si, Ti, Al, Fe+++ ,Fe++ ,Mn, Mg, Ca, Na, K, P, Cr, Ni and sets an index parameter which tells Igpet to multiply these oxides, just before plotting, by:

$$100/(\text{Sum of oxides}), \text{ in which } Fe_2O_3=0 \text{ and } FeO=FeO+.8998*Fe_2O_3.$$

The original data are not changed so you can turn Normalization on and off without getting round off errors. A new parameter, FeO^t, is added. It is total Fe as FeO, normalized to 100%. This new parameter will be removed when you turn Normalization off, unless you have subsequently added other parameters.

If you want to normalize trace elements by the same factor as the major elements answer "Yes" to get a list of data fields. The major elements are preceded with * indicating that they will be normalized. To do the same for any trace elements, double-click the element. When done, click **OK.**

In the Special Diagrams, an XY plot can be normalized to 100% volatile free by adding NMX and/or NMY after the XY diagram descriptor, so the first line of the diagram description begins with XYNMXNMY for the LeBas TAS rock-type diagram (setting SiO_2 and total alkalies to their normalized values.

Resetting the Ferric/Ferrous ratio
Because many data sets present all the Fe as either Fe_2O_3 or FeO, there is a need to apportion the Fe in a reasonable way. For Pearce element ratios and CMAS projections Igpet has a subroutine that uses the logic of Sack et al. (1980) to reset the Fe oxides. If you chose to reset this ratio, you will be asked for a Temperature (Centigrade) and fO_2. The default T, fO_2 are stored in igpref.ini and can be changed in the **Preferences** window under **Miscellaneous**. The values 1150º and -8.16 (the defaults as shipped) are approximately on the NNO buffer.

Irvine and Baragar (1971) based rock identification on the CIPW Norm. They recalculated FeO and Fe_2O_3 using $Fe_2O_3 = 1.5 + TiO_2$. If the analysis value is less than this, no change is made.

In the Minerals subroutine, the charge balance logic of Lindsley and Anderson (1983) is followed to partition the Fe oxides before plotting pyroxenes on the geothermometer.

Extra Param. (File Menu)
Commonly used calculations can be stored here and automatically made, rather than using Igpet's calculator. The data file "EXTRA.DIA" is described in Appendix A. It includes a few standard parameters. The parameter FeO* is $FeO + 0.8998 * Fe_2O_3$ and it has not been normalized. Mg# is $100 * MgO/(MgO + FeO + 0.8998 * Fe_2O_3)$, where the oxides are first divided by their molecular weights. Ba/La and La/Yb are just what they say. There are several built in parameters. Ce* and Eu* are normalized values obtained by log interpolation from adjacent REEs. Density is calculated on a normalized basis, using the method of Bottinga and Weill (1970). Viscosity is crudely estimated after Giordano et al. (2008), using 1000° C and 2 wt% H_2O.

Pearce Param. (File Menu)
The problem of closure in rock analyses (they add to 100% more or less) makes interpretation of traditional Harker (SiO_2) and Fenner (MgO) diagrams inconclusive (see Chayes, 1964). These diagrams allow no simple determination of which minerals or combinations of minerals are being removed (or added) to a magma. The basic problem is that whatever direction SiO_2 is going, most other oxides must perforce go in the other. What is worse is that although a large percentage of what is removed is SiO_2 it usually will go up anyway.

A partial solution to the closure problem is to divide the X and Y variables by a common, highly incompatible or conserved element, like K in arc lavas or Ti in tholeiitic basalts. Explaining specific combinations of oxides that will test for the removal of one or more minerals is outside the scope of this guide. Please refer to Pearce (1968), Russell and Nicholls (1988), Stanley and Russell (1989), Russell et al. (1990), Defant and Nielsen (1990).

To test the utility of Pearce Element Ratio diagrams (PER diagrams), read the file, "BOQUERON.ROC". Fairbrothers et al. (1978) showed that an older suite at Boqueron had a calcalkaline fractionation trend caused by removal of nearly equal proportions of plag and cpx {pl/(cpx+pl)=0.55}; whereas the recent lavas had a tholeiitic trend caused by removal of much more plag than cpx {pl/(pl+cpx)=.72}. Olivine, opx and magnetite play a minor role. This result was obtained tediously by making a great many least squares mixing calculations.
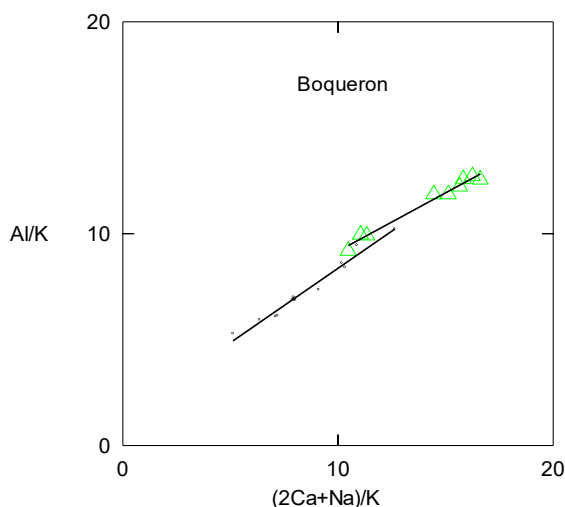
Now test this with a PER diagram. Let X be (2Ca+Na)/K and let Y be Al/K (Russell and Nicholls, 1988). In this projection the slope of the regression should be pl/(pl+cpx) and ol will have no effect. The open diamonds are the early calc-alkaline suite and the small circles are the recent tholeiitic lavas. A filled diamond, not shown above) is a back-arc cinder cone. Use the **Symbols** routine to select one suite and then the other. Make a regression for each. The slope is the pl/(pl+cpx) ratio. The PER diagram method reaches the Fairbrothers et al. conclusion in a flash.

CIPW Norms (File Menu)
The CIPW Norm is familiar to most geologists. Adding a Norm is essential for the Irvine and Baragar (1971) classification scheme, which is covered in one of the special diagram options. Igpet's CIPW is not complete, but it is serviceable for most uses. The normalization subroutine described above does not affect the data that are input to the CIPW subroutine, so, you are asked again if you want to normalize the data to 100% before calculating the Norm.

Rock and Mineral Data Files

Igpet's file reading logic uses tab delimited txt files, an ASCII or flat text file. The file begins with a row of names, one for each column or data field. Columns are separated using tabs. Oxides and other data can be in any order.

Earlier Igpet files used comma delimiters. These files can no longer be read by Igpet. A translation utility, translate.exe, changes the older format to tab delimited text.

Tab delimited data file structure
The first row is the list of column/field names; each subsequent row is an analysis.

dum	Jcode	Kcode	Lcode	sample	SiO[2]	TiO[2]	Al[2]O[3]	etc.
81	1	4	4	PLA7	50.89	.879	20.21	etc.
81	1	4	4	PLA8	etc.			

Each row is read as a single string and then parsed.

Format features
The [2] and [3] in the parameter names signify that these are subscripted variables in plots. Similarly, {87} or {86} define superscripts. The first line has **5 reserved words**, two of which, Sample and Kcode, should be included in any file.

Sample	the sample name, a string variable
Jcode	an integer that can be used to control the symbols in plots.
Kcode	integer variable that is the **default control** for symbols.
Lcode	an integer that can also be used to control the symbols.
dum	placeholder that allows Igpet to ignore any columns not needed.
error	for error bars, the error in with the previous column e.g.

SiO[2] error
  51.3 .513   for a 1% error in SiO_2

Using Igpet's File Operations

From the File Menu click **File Operations**. This menu gives you nine choices.

Print a table
This option allows you to print a list of analyses, where each one is a vertical column.

The table can be sent to: screen (to preview or examine the data set)
                            file   (best option for publication, because you can edit it)

You are first asked "How many columns of data?". Suitable values for the screen and printer are listed. Next, comes a grid that you fill with the number of decimal places for each field. To start this click the edit field in the upper left. All data entry is at that point. Type the first integer, press the Enter key, type the next integer etc. When done click **OK/Save**

The next page asks if you want to calculate a total. If you answer yes, you get the grid again, but this time enter 1 if you want to include the field in the total. When done click **OK/Save.**

Next you get a choice of three output buttons. Select **Screen**. Now the table is printed. If you don't like how it looks on the screen, you can correct the choices you made and print it again. Get it right on the screen before you send it elsewhere.

To stuff more columns on a page, send the output to a file. Pick it up there with a word processor and use a small, monospaced font to allow more columns to be packed onto a page. Trial and error needed here, the number of columns you can squeeze in depends on both the printer and the word processor. **For printing with a word processor it is critical to use a monospaced font.** Proportional fonts cause havoc.

Modify
This is very useful for looking at the data. A grid is presented with all the data. You can move around in the grid and edit any datum by double-clicking and then editing it.

Any changes made here will be reflected in subsequent plots only after **NewX**, **NewY** or **Symbols** has been clicked (depending on what you changed). No change has been made in the original data file on the disk. To change the data file, you must use the **Save** option.

Enter data
If no file has been read, you get a page of instructions when you select this option. The purpose of the instructions is to get a correct list of the data fields you want to enter in the order that Igpet will save them in. The next page allows you to change the order in which you enter the data. This is convenient if your data list (e.g. output from an analytical instrument) is in an odd order. This option should save some mental strain because it allows you to type the data in the order they are listed, but they will be saved in the order you previously specified.

If a file resides in memory and you select "Type in data" you can to add to the data file using the format of that file.

Clear all data
If a file resides in memory, this allows you to clear it out, so you can start fresh.

Save file
Warning except for sample name all text data will be turned to zero. Use a new name!
The file save dialog box opens and you select a new name and or extension.

Add a file (Merge Files)
This option allows you to merge two files that have different (or the same) formats. There is a catch. If the second file has data fields that the first file lacks, these data fields will not be part of the new joint file. This option is useful for adding mineral analyses to a ROC file.

Read the Clipbrd
Small files can be passed between applications via the clipboard. If you have clipped a file in your spreadsheet or word processor, click this button and Igpet will read it. Reading is slow because the clipboard is one large string that has to be parsed. Files larger than 150 by 50 may not fit on the clipboard.

Copy file to Clipbrd
Sends current data file to clipboard, so you can paste it into a spreadsheet.

Import/Export of files

Data files to and from spreadsheets via .txt files
Excel and some other spreadsheets can write **tab delimited txt files**. Use Excel to maintain your data files in Excel's native *.xls format. When you are ready to make some plots, save the data file as a tab delimited text file (a *.txt file). Use your spreadsheet to update data files; it is much more efficient than a text editor or Igpet's crude file operations grid.

Using a word processor to make files
Most word processors have the ability save their work into ASCII files. The file structure needed for Igpet is shown above. It is straightforward to enter the data in the correct order as specified above. If you are going to take this route, by all means try it first on a short file, one or two analyses, until you have the process ironed out.

Pre-designed Diagrams

Igneous petrology is full of specialized plots designed for a variety of purposes. Usually the parameters are linear combinations of major oxides in either wt% or molar terms. There are also many trace element ratios. Several derived parameters are commonly used for the X or Y-axis (e.g. Mg#, Ce*, εNd). Earlier versions of Igpet allowed one to formulate these derived parameters but the logic was awkward. The Text box equation parser, described above, was created to give Igpet the capacity to parse equations and correctly carry out the functions, operations and combinations specified. The new logic, facing the user, is therefore simpler. All the control files that call the equation parser are text files (.txt) that can be modified or added to using a text editor.

Special diagrams (in Diagrams Folder)
Fenner.txt and Harker.txt are multiple MgO and SiO_2 plots respectively. On a printer the eight subdiagrams in each file will be packed into the same page in two rows of four. This is a handy way to make a quick survey of a data set. When you are satisfied with the first diagram, click **Print**. After the plot is sent to the printer buffer, answer **NO** when asked if this is the last plot on the page. End the plot only after the eighth diagram is done.

There are several groups of discrimination diagrams (e.g. basalt, granite, komatiite) which attempt to define the tectonic environment of rock suites or provide useful nomenclature. Most of the discrimination diagrams are reviewed in Rollinson (1993).

IrvineBaragar.txt is the Irvine and Baragar (1971) rock classification scheme.

The construction of specialized diagrams is summarized below.

Mineral Diagrams (in MIN Folder)
Plots for mineral analyses are weakly developed in Igpet. Some simple mineral plots are created

by the control file Miscell.txt in the MIN folder.

The first line has 4 entries separated by tabs. MTRI tells Igpet this is a mineral plot and the shape is triangular. Next is the plot name and then two minerals that are sought for this plot. The next three lines define the left, top and right apices of the triangle. Each line consists of Label-tab-Equation. The subsequent line defines the part of the triangle that is plotted. The six entries are leftmin, leftmax, topmin, topmax, rightmin, rightmax. A topmax of 0.5 creates the familiar quadrilateral shape. The final two lines are empty, just a zero in each. This tells Igpet there are no interior lines and no labels

```
MTRI  Simple Pyroxene Quadrilateral      CPX   OPX
En    MgO
Wo50  CaO
Fs    FeO+MnO
0     1    0     .5    0     1
0
0
```

Igpet will not plot an analysis unless the opx or CPX strings are present in the sample name. It doesn't have to be the entire name, just part of it (e.g. Sal-SA-206 cpx core). There are also mineral strings in the partition coefficient files. So, you should to coordinate your mineral sample names with the mineral strings in Mineral text files the partition coefficient files.

One complex diagram, the Lindsley and Anderson (1983) two pyroxene geothermometer, is included. Fe++/Fe+++ is determined by charge balance in a special subroutine derived from the original publication.

CMAS Projections (in CMAS Folder)
There are many ways to transform the major elements into the four end-members, C, M, A and S. Elthon (1983) provides a lucid review. The textbook "The Interpretation of Igneous Rocks" by Cox, Bell and Pankhurst (1979-Allen and Unwin, London) has good graphical depictions of projections. O'Hara (1976) describes the advantages of "pseudoquaternary isostructural molecular equivalent weight projections". Grove and Baker (1984) suggest that projections should be on an oxide basis, rather than a molar or weight basis. There is no agreement on how best to employ the many projections that exist. Different ones may be suitable for different circumstances. To pursue this, I suggest starting with O'Hara (1976).

The Phase boundaries in the Grove plagioclase projection include the results of Sack et al. (1987). This results in a straighter cpx-ol boundary, near the cpx-ol sideline.

Earlier versions of Igpet had separate CMAS and Projection routines. Now they are combined into a single expression. This is generally the way they are presented in the literature, so as new projections are devised they will be easy to incorporate.

Discrimination and classification diagrams (in Diagrams folder)
DiscrimBasalt.txt, Granite.txt, Komatii.txt, Mantle.txt, Petrol.txt, Irvbar.txt are files containing groups of diagrams that attempt to define (or discriminate) the tectonic environment of rock suites or provide useful nomenclature. Irvbar.txt is the Irvine and Baragar (1971) rock classification scheme. The plotting parameters for the DiscrimBasalt file are mostly from Rollinson (1993). For proper use, these discrimination diagrams should be used only in conjunction with Rollinson (1993) or the original references!

Two diagram files cover the IUGS Cation NORM classification, based on Streckeisen and Le Maitre (1979) and the IUGS Modal classification (Streckeisen, 1976). The first file requires you to add a CIPW norm using the Barth-Niggli Cation Norm option (look in the File menu). The second is based on Petrography, real point counts. This should not be used with the CIPW Normative minerals. Instead, add columns of data in your spreadsheet with mineral modes (and combinations of minerals). The mineral names I used are: plagioclase, orthopyroxene, clinopyroxene, olivine, hornblende, quartz, feldspathoids (a combination- see ref.), alkali_feldspar (another combination).

Spider Diagrams (Spider.txt in Controls Folder)
Basic references on Spider Diagrams are Thompson (1982), Thompson et al. (1984), and Wilson (1989). The special buttons for spider diagrams are:
Repick   means go back to the list of analyses and pick a new subset.
New Spi.   returns you to the list of diagrams (Spider.txt is in the Controls folder).
Y-Scale   lets you reset the y-axis limits and switch to a linear axis.

Notes on some calculations

Mixing and Mixing
In the Mix option in XY plots Igpet's logic follows Langmuir et al. (1977) and calculates the coefficients of the hyperbola equation from two endpoints. This allows the mixing line to be extended beyond the selected endpoints. For isotopic ratios the ppm value of the element is sought in the data fields. If it isn't found the routine terminates. For Sr, the routine uses the ppm value, the relative abundances of non-radiogenic Sr isotopes and the 87/86 ratio to calculate ppm ^{87}Sr and ppm ^{87}Sr. The values for each endpoint go into the equation for determining the coefficients of the hyperbola. For Nd and Pb the same routine is followed. In plots of Pb ratio versus Pb ratio, the mixing curve should be a line because ^{204}Pb is the denominator on both axes.

The mixing line, calculated in the model option, is identical to the line in the Mix option between the endpoints, but can't extend beyond them. In the model option the program makes small steps between the endpoints and calculates each element in the mix separately. The hyperbola equation is not involved.

A third mix option is available in Spider diagrams, see above.

AFC Modeling
This option will be unclear unless you have a copy of DePaolo (1981) as a guide. The file, DEPAOLO.ROC, will allow you to reproduce DePaolo's figure 3. Not all of DePaolo's equations are included in Igpet.

Adding tie lines
The parameter that controls symbols (usually Kcode) uses integers between 0 and 16. To draw a tie line between two points, let the symbol parameter of the second point be a negative number. The symbol routine really looks at the absolute value of the integer and uses the sign to key a pen up before moving command.

Common Problems

Zeros are not plotted
In all the graphs X, Y, or Z values of zero are not plotted, because in most data sets 0 means not determined or below detection limit.

Errors in a data file
If Igpet fails to completely read a file, the matrix limits may have to be changed or the file may be corrupt. A corrupt file has either too many or too few elements in some analysis. To find out where the problem is, go immediately to the File Operations menu and select Modify. You should be able to track down the error by locating where the data become out of place. Sometimes the only error is a few invisible extra lines or spaces at the very end of a file. When you have located the error, use Notepad to fix the problem.

Mixing.Exe

This program makes petrologic mixing calculations using least squares regression of the major elements, after Bryan et al., (1969). Trace element calculations are made, based on the major element solution. Many researchers use this technique to test the plausibility of models of crystal fractionation or magma mixing. What criteria to use to judge whether a model is permissible is debatable and can vary with the problem being addressed. In general, the residuals (the difference between observed and calculated) should be within analytical error. However, low residuals are no guarantee that the model is successful. The high degree of covariation of major elements really means that there are few degrees of freedom and it allows successful appearing fits of some nonsense models. The best you can say of a model with low residuals is that it has not been rejected, but it certainly can not be proved with this technique. The good news is that a great many models fail and can be rejected, so this a valuable tool within its limits.

To start MIXING, click on the MIX icon.

MIXING starts with its main menu. First read a partition coefficient file (.PC.txt), then a weighting function for oxides file (.wt.txt), a rock file and a mineral file. You can read new mineral, rock or PC.txt files at any time.

The partition coefficient files hold the partition coefficient data needed for trace element calculations. The weights files hold the weighting values for the major oxides. Even if you are not interested in trace element calculations, select a PC.txt file and weight file. Different partition coefficient files should be created for different types of rock suites. Select the partition coefficient file you want (e.g. Gill.PC.txt)

A button at the lower left lets you list the partition coefficient and weighting data. Check it for correctness. The mineral abbreviations at the top of the matrix are strings that will be looked for in each sample name in the mineral file you read. These strings have to be somewhere in the mineral names for MIXING to tie a set of partition coefficients to the mineral. In Gill.PC.txt plagioclase is "pl". Thus, a plagioclase in a mineral file has to have "pl" somewhere in its name to have the correct partition coefficients tied to it (e.g. "CN9PLAN75").

The weight for each oxide data allows you to reduce the effect of the overwhelming predominance of SiO_2 and Al_2O_3 in most analyses. Before least squares calculation, each oxide will be multiplied by its "weight". The analyses are then printed in un-weighted form, but the residuals and sum of squares of residuals are weighted values. If a weight file has weights of 0.4 for silica and 0.5 for alumina, there will be a discrepancy for these oxides between the difference between the Observed and Calculated magmas and the calculated (weighted) residual. You can change the weights to 1.0 to eliminate this, but then you will be giving silica and alumina more control over the result. You can also give an oxide a weight of 0.0 and it will not contribute to the least squares solution. Fe_2O_3 is multiplied by 0.8998 added to FeO and subsequently ignored.

Now all the data are in place and you can begin making models. If you are trying Cerronego.txt and cerronegro.min, you can find published examples in Walker and Carr (1986). The usual model is Fractional Crystallization (Fract. Xtl.)

First, pick minerals. It's unwise to pick two or more of the same minerals, e.g. two olivines.
Second, pick a daughter
Third, pick a parent. (You can reverse these if you prefer.)

the general equation is:

parent = (C1, C2, C3,..., Cd) * (min1, min2, min3,...., daughter)

Mixing solves for the coefficients (C's).

The result is seen as soon as you finish your selection. Output goes first to the screen, but you can send a copy to the printer, a text file or a corrected rock file. The last option allows you to build a ROC file of fractionation corrected data, which is useful for trace element modeling.

If you are familiar with an older version of Mixing, there is one significant change. Mixing now reads the Oxide and Oxide weights in the weighting files as entire lines. These data used to be fixed to 11 oxides in a particular order. Now the order is flexible and up to 15 oxides can be used AS LONG AS ALL ARE ON THE SAME LINE. THE LOGIC ONLY READS ONE LINE OF OXIDES. The weights must be on a separate line. This change is not a big deal, but it allows Cr_2O_3 and NiO to be added. Fe_2O_3 should be eliminated because the program automatically converts all Fe_2O_3 to FeO. The order of the oxides in this line is the order they will be printed in the output.

Appendix A: Control Files

IGPREF.INI and **Igpetdata.txt**
These files control the IGPET system. You should modify **IGPREF.INI** using the **Preferences** menu and the resize matrix and font menus.

Igpetdata.txt is basic data in tab delimited rows. Part of the file is shown below.

60.084	79.899	101.96	159.69	71.846	70.937	40.311	Mol wts of 14 oxides
1	1	2	2	1	1	1	number of cations
SiO2	TiO2	Al2O3	Fe2O3	FeO	MnO	MgO	oxide name
Si	Ti	Al	Fe	Fe	Mn	Mg	ppm name
4674	5995	5292	6994	7773	7745	6028	convert to ppm
26.75	22.45	37.8	44.4	13.94	14	12.32	partial molar volumes
%AN	Q	or	ab	an	lc	ne	CIPW norm names
-2.15	0	-8.35	0	-4.5	0	-5.44	Sack et al 1980 to reset Fe++/FE+++

{87}Sr/{86}Sr   labels Igpet will recognize and may adjust
{143}Nd/{144}Nd   e.g. convert 87sr/86sr   to {87}Sr/{86}Sr
{206}Pb/{204}Pb
{207}Pb/{204}Pb
{208}Pb/{204}Pb
{10}Be
Be
Li
etc

DEFAULT_NRM.txt normalization used in S-Norm in button calculator, set the file you want in the preferences window. Note that the first line is a comment

'Sun and McDonough 1989 primitive mantle
Cs   .0079
Tl   .005
Rb   .635
Ba   6.989
W   .02
Th   .085
U   .021
Nb   .713
Ta   .041
K   250

Page.txt controls where Igpet draws its plots. There are 16 options.

```
8000    10250   'page width-height in Portrait mode in 1000's of an inch
16
Portrait        2000   4000   7000   7500    XYL
Portrt-Upper    2000   6500   7000   10000   XYL
Portrt-Lower    2000   2000   7000   5500    XYL
Portrt-UUL      1400   7200   3900   8950    -YL
Portrt-MUL      1400   5300   3900   7050    -YL
Portrt-LML      1400   3400   3900   5150    -YL
Portrt-LLL      1400   1500   3900   3250    XYL
Portrt-UUR      4100   7200   6700   8950    -YR
Portrt-MUR      4100   5300   6700   7050    -YR
Portrt-LMR      4100   3400   6700   5150    -YR
Portrt-LLR      4100   1500   6700   3250    XYR
Lndscp-Page     2500   2500   9500   7500    XYL
Lndscp-LL       1500   1700   5000   4200    XYL
Lndscp-LR       5500   1700   9000   4200    XYR
Lndscp-UL       1500   5100   5000   7600    XYL
Lndscp-UR       5500   5100   9000   7600    XYR
```

Symbol Files or sym files

TTSYMS.SYM stands for two-toned symbol file. Widths and lengths are in 1000s of an inch. The first two lines are special, the rest of the lines have a common format, one (or more) line per symbol. Circles and polygons have slightly different formats, but both begin with 6 integers that specify the color of the line, first 3, and the fill, second 3. Polygons have an integer that specifies the number of points in the polygon.

```
.7,13  scale factor for symbols, thickness of outer line in 1000s of inch
19    number of symbols in file
0,0,0,0,0,0,"CIRC",1,30,30
[red,green,blue]line color,[red,green,blue] fill color, circle, 1 apex, radius of 30, dummy
0,170,85,255,255,255,"POLY",4,130,-74,0,152,-130,-74,130,-74
[red,green,blue]line color,[red,green,blue] fill color, polygon, 4 apexes, x1,y1,x2,y2,etc (triangle)
0,170,85,75,255,175,"FPOLY",4,130,-74,0,152,-130,-74,130,-74
same as previous but polygon is filled
more examples follow
0,0,200,255,255,255,"POLY",5,-112,-112,112,-112,112,112,-112,112,-112,-1120,0,200,175,175,255,"FPOLY",5,-112,-112,112,-112,112,112,-112,112,-112,-112
200,0,200,255,255,255,"POLY",5,100,0,0,160,-100,0,0,-160,100,0
200,0,200,245,0,245,"FPOLY",5,100,0,0,160,-100,0,0,-160,100,0
225,0,0,255,255,255,"CIRC",1,112,112
225,0,0,255,0,0,"FCIRC",1,112,112
```
several lines deleted
```
255,128,0,255,200,0,"FPOLY",17,50,50,50,100,0,150,-50,100,-50,50,-100,50,-150,0,-100,-50,-50,-50,-50,-100,0,-150,50,-100,50,-50,100,-50,150,0,100,50,50,50
0,0,0,0,0,0,"CIRC",1,40,40
```

0,0,0,15,"tickpen color-RGB,width"
0,0,0,20,"mixmodpen color-RGB,width"
255,255,255,99,"pagecolor"
255,255,220,99,"boxcolor"
0,0,0,99,"textcolor"

SPIDER.Txt This file controls spider diagrams.

First line is: **title, normalization factor**
Second line is: **15   x   1   1000   15 elements, x=no double norm, y axis min, y axis max**
Third line is element list
Fourth line is normalization factor

Sun+McDon. 1989-REEs	Chondrites											
15	x	0.7	500									
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm
0.237	0.612	0.095	0.467	1	0.153	0.058	0.2055	0.0374	0.254	0.0566	0.1655	0.025
Nakamura 1974-REEs		Chondrites										
15	x	1	1000									
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm
.33	.865	.112	.63	1	.203	.077	.276	.047	.343	.07	.22	.03
Sun+McDon. 1989			Primitive Mantle									
22	x	1	1000									
Cs	Rb	Ba	Th	U	Nb	K	La	Ce	Pb	Pr	Sr	P
.0079	.635	6.989	.085	.021	.713	250	.687	1.775	.071	.276	21.1	95
Sun+McDon. 1989			Primitive Mantle double norm									
23	Yb=10	1	1000									

NOTE double norm to Yb and set all normalized Yb values to 10.

EXTRA.txt

This file has parameters that are automatically calculated and added to the variable list when the menu item, file operations - extra is selected. Each extra parameter has three entries; the label is first, the odd string zerosin or nozeros is second and the equation is third. In some equations the lack of a component makes the resulting expression meaningless. For example, if Nb+Ta is called for and the data set contains Nb but only some Ta values, then the Nb+Ta equation will yield a false result wherever Ta is absent, thus "nozeros" is appropriate. On the other hand, if the parameter is FeO +0.8998*Fe2O3, there are many data sets that lack one or the other of these oxides so one uses "zerosin." The CIPW norm famously sets some normative minerals to zero so many combinations of CIPW normative minerals (e.g. an+ab+.6*ne) require "zerosin."

The extra routine adds several fixed items as well, Ce*, Eu*, Nb*, density, after Bottinga and Weill (1982) on a water-free, 1 atm, 1200° C basis and viscosity with 2%water at 1000° C after Giordano et al. (2008).

FeO*	zerosin	FeO+Fe2O3*.8998
Mg#	zerosin	MgO*2.481/(MgO*.0248+FeO*.013918+Fe2O3*.012523)
Ba/La	nozeros	Ba/La
La/Yb	nozeros	La/Yb
U/La	nozeros	U/La
Ba/Th	nozeros	Ba/Th
Zr/Hf	nozeros	Zr/Hf
Zr/Nb	nozeros	Zr/Nb
eNd	nozeros	"{143}Nd/{144}Nd"*19505.344464383241-10000

Nb* is an interpolation between K and U.

K is K_2O times 8301.

K_N is K/250

U_N is U/0.021

Nb_N will be the interpolated value/0.716

Note: the 250, 0.021 and 0.716 are from the 'primitive mantle' of Sun and McDonough (1989)

$Log(Nb_N) = (Log(K_N) /2.303 + Log(U_N) / 2.303)/2$

$Nb* = 0.716 * Exp(2.303 * Nb_N)$

Diagrams Folder

These files allow for predefined diagrams. The control data differentiate XY vs. TRI diagrams, define the X, Y, and Z parameters, define dimensions, interior lines and labels. Some diagrams are complex. Look at some examples, drawn from various examples, to learn how to mimic them. Replace "XY" with "XYSMALL" if you want small fonts for interior labels. The delimiter, separating fields, is a tab.

The first line consists of 4 entries: diagram control, the label, the source and a comment. The first entry is very important; the others are not. The next three lines define the left, top and right apices of the triangle. Each line consists of Label-tab-Equation. The subsequent line defines the part of the triangle that is plotted. The six entries are leftmin, leftmax, topmin, topmax, rightmin, rightmax. Next comes an 18 which tells Igpet that there are 18 interior line segments. The next 18 lines are left, top pen control, where 1 is down and zero is up. The next line is an 8 telling Igpet there are 8 labels. The next 8 lines are the left, top values and the label.

It is important that the oxide or element names used here are the same ones used in the data files. Igpet will compare names on an all uppercase basis with {, }, [,] stripped out.

```
TRI      Zr-Ti/100-Y*3    Pearce+Cann 1973        5.1 Thol. basalts with CaO+MgO 12-20%
Zr       Zr
Ti/100   TiO2*59.95
Y*3      Y*3
0        1        0        1        0        1
18
.555     .24      0
.59      .28      1
.385     .50      1
.24      .48      1
…………………..several lines cut
8
.5       .2       C
.4       .4       D
.27      .37      A
.35      .3       B
-.1      .75      Island-arc A B
-.1      .60      Ocean-floor B
-.1      .45      Calc-alkali B C
-.1      .30      Within-plate D
```

This triangular plot adds ZEROSIN to the diagram control string, allowing forgiveness if FeO or Fe2O3 is not measured. The diagram label is AFM.

```
TRIZEROSIN    AFM    thol vs calc-alk    Irvine+Baragar 71
Alk      Na2O+K2O
FeO*     FeO+Fe2O3*.8999
MgO      MgO
0        1        0        1        0        1
……
```

The next example is an X-Y plot. It has the same first line as the TRI plot: the diagram control, the label, the source and a comment, in this case referring to a diagram in Rollinson's book.

The next two lines are: the Xaxis label-tab-equation and: Yaxis label-tab-equation.

The next two lines control the axes, first x and then y.

The initial zero says this is not a log plot. The 0 tab 200 sets the range of the x-axis, the two 100s tell Igpet that the tick step is 100 and the label step is 100.

An axis control line is: linear=0 or log=1, beginning of range, end of range, tick-step, label-step

```
XY      Zr vs Ti Pearce+Cann 1973        5.2a Thol. basalts with CaO+MgO 12-20%
Zr      Zr
Ti      TiO2*5995
0       0       200     100     100
0       0       14000   1000    5000
21
135     7100    0
113     7400    1
89      7400    1
……..many lines cut   then 5 labels with: x tab y tab label
5
15      2000    IAT
55      6000    B
125     4000    Calc-alkali basalt
100     9000    MORB
20      12000   B=MORB+C-A bas+IAT
```

The following example includes division (A/B). This plot must have ZEROSIN in the diagram control field because ne is usually zero. Note that the x-axis is reversed going from 100 to 40.

```
XYZEROSIN      %An-Al2O3        thol vs calc-alk    Irvine+Baragar 71
AN      an*100/(an+ab+.6*ne)
Al[2]O[3]       Al2O3
0       100     40      10      10
0       10      25      1       5
7
40.000  15.200  1
50.000  16.000  1
60.000  16.800  1
70.000  17.600  1
80.000  18.400  1
90.000  19.200  1
100.000 20.000  1
2
90      15      Tholeiitic
90      22      Calc-Alkaline
```

The following example draws a box shape and uses a log scale for x and y. For a log scale the tick-step and label-step are set to zero. They need to be included even thought they are ignored.

XY BOX		Y+Nb vs Rb		Pearce et al. 84
Y+Nb	Y+Nb			
Rb	Rb			
1	2	2000	0	0
1	1	2000	0	0
7				
2	80	0		
55	300	1		
400	2000	1		
55	300	0		
50	1	1		
51.5	8	0		
2000	400	1		
4				
5	750	syn-COLG		
300	600	WPG		
6	3	VAG		
300	8	ORG		

MIN folder

The format of these files is similar to the triangular diagram files.
The last two entries in the first line define which mineral to plot.

SMTRI	Feldspar Triangle PL		FS		
Ab	Na2O				
An	CaO+MgO				
Or	2*K2O				
0	1	0	1	0	1
0					
0					
MTRI	Simple Pyroxene Quadrilateral		CPX	OPX	
En	MgO				
Wo50	CaO				
Fs	FeO+MnO				
0	1	0	.5	0	1
0					
0					

CMAS folder

The format of these files is slightly different from that for the triangular files for regular diagrams. The diagrams control parameter CTRI tells Igpet that this is a CMAS projection with three extra data, the final apex scaling values. These numbers follow the apex labels. They are all 1 in this case (molar) but can be in weight or oxygen units.

```
CTRI    Plag. Proj.        Walker et al 79 Sack et al 87        mole
OL      1        .5*Al2O3-.5*Fe2O3+.5*FeO+.5*MnO+.5*MgO-.5*CaO-.5*Na2O-.5*K2O
DI      1        CaO+Na2O+K2O-Al2O3
SIL     1        SiO2-.5*Al2O3+.5*Fe2O3-.5*FeO-.5*MnO-.5*MgO-1.5*CaO-5.5*Na2O-5.5*K2O
0       1        0        1        0        1
27
.4535   .708     0
.4169   .58802   1
.3825   .472     1
.3457   .379     1
….  Many lines cut
1
.55        -.07     Opx
```

This example includes "zerosin" in the diagram control field because many analyses lack Cr_2O_3 or NiO. This also gives an example of scaling by wt% and the triangle is shaved in all three axes.

```
CTRIzerosin     M2S to CS60-A30-MS      O'Hara 1968       WT
CS-60   116.16  CaO+Na2O*2+K2O*2-P2O5*3.333
A-30    101.96  TiO2+Al2O3+Cr2O3+Fe2O3+Na2O+K2O
MS      100.4   SiO2*2+TiO2-FeO-MnO-NiO-MgO-CaO*2-Na2O*8-K2O*8+P2O5*6.666
0       .6      0        .3       .4       1
2
.54     0       0
.275    .245    1
4
.58     -.03    CMS[2]
.12     .09     AV
.29     .255    Ol-Pl
.005    .245    - M[3]AS[3]pyrope
```

PEARCE.txt

Pearce diagrams are based on element proportions, E.

$\quad$ E= (wt% * # of cations)/molecular wt.

These are calculated for all the oxides in the Pearce subroutine. Pearce.txt consists of meaningful combinations of these element proportions. Consult Stanley and Russell (1989) for the appropriate use of these parameters. In the file, each line consists of label-tab-equation.

```
K           K2O
Ti          TiO2
P           P2O5
Si          SiO2
Al          Al2O3
0.5(Mg+Fe)              0.5*FeO+0.5*MgO
OL+CPX+PL               1.5*CaO+.25*Al2O3+0.5*FeO+0.5*MgO+2.75*Na2O
(Ca+.5Na-.5Al)   CaO+.5*Na2O-.5*Al2O3
(2Na+Al)                2*Na2O+Al2O3
(2Ca+Na-Al)             2*CaO+Na2O-Al2O3
(Si-.25Al-.5FM-1.5Ca-2.75Na)      SiO2-.25*Al2O3-.5*FeO-.5*MgO-1.5*CaO-2.75*Na2O
(-Si+.5Al+FM+Ca+2.5Na)                  .5*Al2O3+FeO+MgO+CaO+2.5*Na2O-1*SiO2
(.5FM+2Ca+3Na)          .5*FeO+.5*MgO+2*CaO+3*Na2O
(2Ca+3Na)               2*CaO+3*Na2O
(.5FM+1.5Ca)            .5*FeO+.5*MgO+1.5*CaO
(2Ca+Na)                2*CaO+Na2O
```

Partition Coefficient files

These files are control files for MIXING and modeling in Spiderplots. They have the partition coefficient data. Gill1981.PC.txt, shown below, is a tab delimited file.

el/min	PL	CPX	OPX	OL	HB	MT	GA	IL
K	0.11	0.02	0.01	0.01	0.33	0.01	0.01	0.01
Rb	0.07	0.02	0.02	0.01	0.05	0.01	0.01	0.01
Sr	1.8	0.08	0.03	0.01	0.23	0.01	0.02	0.01
Ba	0.16	0.02	0.02	0.01	0.09	0.01	0.02	0.01
Zr	0.01	0.25	0.1	0.01	0.4	0.4	0.5	0.4
Ni	0.01	6	8	58	10	10	0.6	10
Cr	0.01	30	13	34	30	32	22	32
V	0.01	1.1	1.1	0.08	32	30	8	30

Weight files

These files are control files for MIXING. They have the weighting scheme for the oxides. Default.wt.txt, shown below, is a tab delimited file.

SiO2	TiO2	Al2O3	FeO	MnO	MgO	CaO	Na2O	K2O	P2O5	NiO	Cr2O3
0.4	1	0.5	1	1	1	1	1	1	1	1	

Appendix B: Data Files

COTLO.ROC contains glasses that were formed in equilibrium with Plag-Cpx-(Ol or Opx). These glasses trace the 1 atm pseudo- quaternary cotectic that exists at the intersection of the primary phase volumes of these minerals. There is a problem in locating this intersection because additional components, especially K_2O and Na_2O, appear to cause large shifts in the location of this intersection. Different CMAS projections cause different shifts. The problem is to determine how much of the shift is real and caused by thermodynamic effects and how much is an artifact of projection. This is an important problem that needs to be resolved in order to better interpret real rocks projected into these diagrams.

The different Key numbers in this file stand for different data sources.

key	symbol	ref.
1.	open triangle	Walker et. al., 1979
2.	filled triangle	Grove and Bryan, 1983
3.	open box	Baker and Eggler, 1983
8.	filled circle	Grove et al., 1982

COTHI.ROC contain glasses that were in equilibrium with a dry peridotite sandwich at various pressures. For a complete discussion read Takahashi and Kushiro (1983), the source of most of the data. One data point, plotted as a "X", is from Baker and Eggler (1983). This point represents about 8 kb and an unspecified small per cent H_2O. It was not in equilibrium with a peridotite sandwich. Because of the water and the type of experiment, it is not strictly comparable to the rest of the data.

The different Key numbers refer to pressures.

Key	symbol	pressure (kb)	1 Gpa=10 kb
1.	open triangle	5	0.5
2.	filled triangle	8	0.8
3.	open box	10	1.0
4.	filled box	10-10.5	1.0-1.05
5.	open diamond	20	2.0
6.	filled diamond	25	2.5
7.	open circle	30	3.0
8.	filled circle	35	3.5
11.	X	8 (wet)	0.8 (wet)

VGGP.TXT   MORB glass data set provided by Melson et al. (1977). It is a large file of high quality probe analyses of mid ocean ridge glasses from dredge hauls.

Several other data files refer to studies of Central American volcanoes.

FUSAMA.TXT
      Fuego   key=1, see: Chesner and Rose (1984)
      Santa Ana   key=7, see: Carr and Pontier (1981)
      Masaya   key=3, see: Walker et al. (1993)

CERRONEG.TXT
      Cerro Negro volcano in Nicaragua, see: Walker and Carr (1986)

CN.MIN
      see above: this file has mineral analyses from Cerro Negro volcano, Nicaragua

IZALCO.TXT
      see: Carr and Pontier (1981) on Izalco volcano, El Salvador

BOQUERON.TXT
      see: Fairbrothers et al. (1978) on Boqueron volcano, El Salvador

CENTAM.TXT
      see: Carr et al. (1990)

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