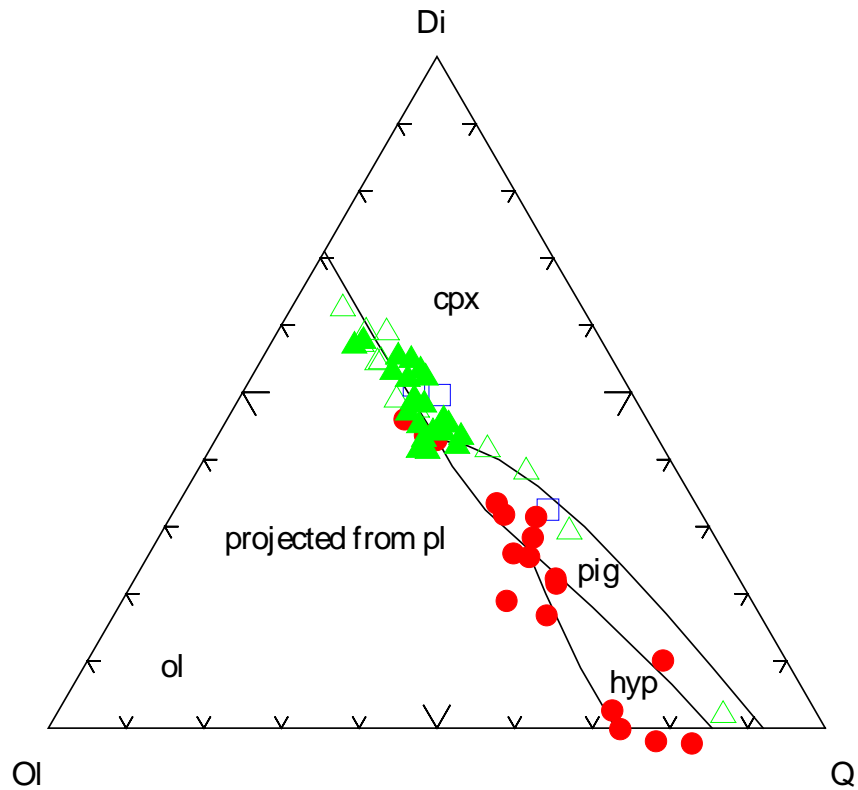


Igpet for Windows
Copyright January 9, 2000

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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, June 2005

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

Upgrade Notes, February 2005

Added a Legend and many smaller improvements and repairs

Upgrade Notes, March 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.

Upgrade Notes, June 2002

Substantial improvements to make Igpert work with Windows XP. Added several more discrimination diagrams and reconfigured several dgm files.

Upgrade Notes, April 2001

Repaired CoDoPo option in Spider modeling. Added a few more dgm files. Fixed minor errors.

Upgrade Notes, March 2000

Igpert uses windows metafiles (.WMF) to transfer graphics to the clipboard and store them on a disk. Earlier Igpert versions relied on a background page to keep aspect ratios in place. This backpage is now an option because it was difficult to remove it in MS PowerPoint and MS Word. Not including a backpage allows Igpert plots to occupy a smaller footprint on a Word page, just the diagram and an inch or so of surrounding space. Word or PowerPoint can then add additional comments on top.

Acknowledgments

My wife and son put up with a lot, allowing me to work on this. My colleagues and semi-willing beta testers, Mark Feigenson, Claude Herzberg, Lina Patino, Karen Bemis and many others repeatedly demonstrate uncanny ability to locate bugs within minutes of getting a "final" version. Over the years several geoscientists have found bugs for me and suggested or provided useful additions. This is a major way that Igpert improves.

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Installing Igpet

Igpet will not work on Windows 3.1. Install it only on a 32-bit system, such as Windows 95 and higher. A setup program, **SetupIgpet05.exe**, installs Igpet. All of Igpet's control files and all the data files shipped with Igpet will be copied to a directory, normally Igpet205, in Program Files.

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: Igpet05. 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. 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 includes a primitive calculator.

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.

A text box, below the calculator, allows you to directly enter simple equations, bypassing the calculator. The recursion routine is not yet smart enough to handle Log(xx), but otherwise seems fairly robust. It is experimental (June 05), so please report problems.

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.

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.

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 flash 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 flash 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.

Edit Menu

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 Iqpet 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. A symbol is eliminated by clicking on the adjacent check box. To select just the Santa Ana data, note the position of the open red circles. Click **Deselect All**, 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.

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 Iqpet 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 make symbols more visible on laptop screens. It also allows you to remove the effects of a black and white printer's effort to reproduce color by drawing dithered shades of gray. Some of these effects are pleasant, but others are ugly. **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.

Three edit fields for line widths allow you to control how fat the lines are in Igpct. The useful range is from 1 to 15 or 20. The colored margins of symbols may be invisible on black and white printers because of dithering. 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.

Set Limits to exclude some data

The **Set Limits** option in the **Edit Menu** allows you to filter your data through two possible windows. 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, so click on **Set Limits** to eliminate them. A list of parameters appears. Double-click on SiO₂. For a lower limit enter 0, for an upper limit enter 58. For the second limit select Quit or OK. A graph without the high silica points will now appear.

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 file called "Stat.ig". 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 **Set Limits** button 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. $\text{Na}_2\text{O}+\text{K}_2\text{O}$, $\text{FeO}+.8998*\text{Fe}_2\text{O}_3$, 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 I now use it 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 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 plots

Elaborate partial melting and simple crystallization models can be performed when a spider diagram is plotted. This requires partition coefficient files (*.pcs), 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 look for 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).

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 is best at modeling melting processes. You start by selecting a model, e.g. **Batch Melt**, then you select whether melting is modal or non-modal (Pi's <> Di's). Finally you get to a window that allows you to pick a partition coefficient file (a pcs file), a mantle mode, a melt mode (if non modal melting), and a set of % melts. You can run the melt equation forward (the default) or backward by toggling radio buttons. When all is set, click the **Make Calculations** button, the bulk D's will appear, 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 buttons of the lower left side of the main window. For printing, the colored backgrounds can waste a lot of ink on drafts, so a 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 do not pass unscathed through the Clipboard or a Windows metafile (WMF) and then onward to a word processor or graphics program. 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 90° which works for HP LaserJets in normal configuration. HP inkjet printers prefer the more logical value of 270°. Make changes in the **Preferences** window and be sure to save the new preferences!

Clipboard from Edit Menu

The clipboard is an easy way to transfer a diagram to a draw program or word processor. The **Copy to clipboard** option in the **Edit menu** option asks you to choose between **Diagram** and **Diagram and background page**. Usually, the diagram option is best. However, if you want to sequentially copy several diagrams onto specific sections of a page, use the background page option. However, when pasting into a draw program, you will have to ungroup each successive diagram and remove its background page.

To see your diagram on the clipboard, activate the Windows Clipboard Viewer. If you have a diagram on the clipboard and want to place it in a Microsoft Word document, move the cursor to where you want it, then open the Draw window (its symbol is the triangle, circle and box). Paste the diagram into the Draw window, where it can be edited. You can just paste the diagram in the Word. 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 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 K₂O 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) and Pearce element ratios (Pearce, 1968) are a way of reducing the problem.

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 Igpert to multiply these oxides, just before plotting, by:

$100/(\text{Sum of oxides})$, in which $\text{Fe}_2\text{O}_3=0$ and $\text{FeO}=\text{FeO}+.8998*\text{Fe}_2\text{O}_3$.

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, 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, move to Quit at the end or beginning and double-click, or click **OK**.

Resetting the Ferric/Ferrous ratio

Because many data sets present all the Fe as either Fe₂O₃ or FeO, there is a need to apportion the Fe in a reasonable way. For Pearce element ratios and CMAS projections Igpert 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 fO₂. The default T, fO₂ are stored in igpref.ini and can be changed in the **Preferences** window under **Miscellaneous**. The values 1150° 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 Fe₂O₃ using $\text{Fe}_2\text{O}_3=1.5+\text{TiO}_2$. 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)

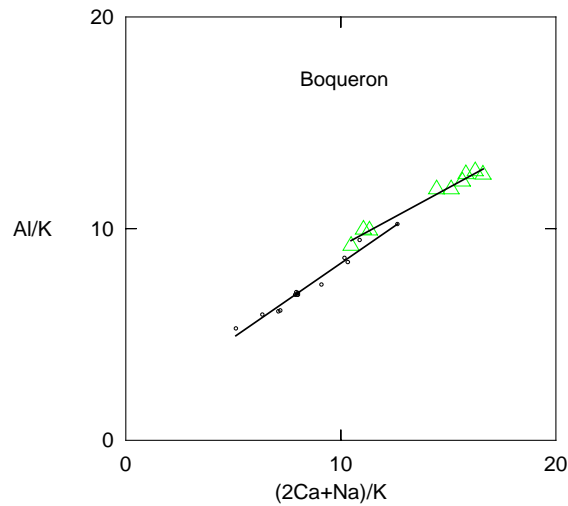
Commonly used calculations can be stored here and automatically made, rather than using Igpet's calculator. The data file "EXTRA.DIA" is described in Appendix A. It includes a few standard parameters. The parameter FeO* is $\text{FeO} + 0.8998 * \text{Fe}_2\text{O}_3$ and it has not been normalized. Mg# is $100 * \text{MgO} / (\text{MgO} + \text{FeO} + 0.8998 * \text{Fe}_2\text{O}_3)$, where the oxides are first divided by their molecular weights. Ba/La and La/Yb are just what they say. There are three 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). It will always be last on the list of extra parameters.

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 $\{\text{pl}/(\text{cpx} + \text{pl}) = 0.55\}$; whereas the recent lavas had a tholeiitic trend caused by removal of much more plag than cpx $\{\text{pl}/(\text{pl} + \text{cpx}) = 0.72\}$. 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 $(2\text{Ca}+\text{Na})/\text{K}$ and let Y be Al/K (Russell and Nicholls, 1988). In this projection the slope of the regression should be $\text{pl}/(\text{pl}+\text{cpx})$ 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 $\text{pl}/(\text{pl}+\text{cpx})$ 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.

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 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 its 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.

Notes on Applications

Multiple diagrams per page

Fenner.DGM and Harker.DGM are multiple MgO and SiO₂ plots respectively. On a printer the eight sub diagrams in each file will be packed into two rows on the same page. 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, answer **NO** when asked if this is the last plot on the page. End the plot only after the eighth diagram is done.

DiscrimBasalt.DGM, Granite.DGM, Komatii.DGM, Mantle.DGM, Petrol.DGM, Irvbar.DGM etc. are groups of diagrams that attempt to define (or discriminate) the tectonic environment of rock suites or that provide useful nomenclature. Irvbar.DGM 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 DGM files cover the IUGS Cation NORM classification, based on Streckeisen and Le Maitre (1979) and the IUGS Modal classification (Streckeisen, 1976). The first DGM file requires you to add a CIPW norm using the Barth-Niggli Cation Norm option (look in the File menu). The second DGM 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).

Mineral Diagrams

Some simple mineral plots are created by the control file MINS.DIA. In the file, MINS.DIA, you can choose two minerals to be plotted in the diagram. You enter string variables like OPX or cpx

(the logic is case insensitive) near the beginning of the plot definition. Igpet will not plot anything 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 PCS files. So, you should to coordinate your mineral sample names with the mineral strings in MINS.DIA and the PCS files.

One complex diagram, the Lindsley and Anderson (1983) two pyroxene geothermometer, is included. It is limited to cpx and Fe⁺⁺/Fe⁺⁺⁺ is determined by charge balance.

CMAS Projections

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.

Spider Diagrams

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 available diagrams (data is in SPIDER.DIA). |
| Y-Scale | lets you reset the y-axis limits and switch to a linear axis. |

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. 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 ⁸⁷Sr and ppm ⁸⁶Sr. These 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 ²⁰⁴Pb 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 (PCS), then a weights for oxides file (MWT), a rock file and a mineral file. You can read new mineral, rock or PCS files at any time.

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

A button at the lower left lets you list the PCS and MWT 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.PCS 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 allow you to reduce the effect of the overwhelming predominance of SiO₂ and Al₂O₃ in most analyses. Before least squares calculation, each oxide will be multiplied by its "weight". The analyses are then printed in unweighted form, but the residuals and sum of squares of residuals are weighted values. If a MWT 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. Fe₂O₃ 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 Cerroneg.ROC and CN.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:

$$\text{parent} = (C1, C2, C3, \dots, Cd) * (\text{min1}, \text{min2}, \text{min3}, \dots, \text{daughter})$$

and 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 MWT (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 Cr₂O₃ and NiO to be added. Fe₂O₃ should be eliminated because the program automatically converts all Fe₂O₃ 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 IGPET.DAT

Modify **IGPREF.INI** with the **Preferences** menu and resize matrix menu. **IGPET.DAT** is data, shown below, that can be left as is.

```
60.0848,79.899,101.961,159.692,71.846,70.9374,40.311,56.0794,61.979
94.2,141.95,74.71,151.9902,18      molecular wts of 14 oxides
1,1,2,2,1,1,1,1,2,2,2,1,2,2      # of cations for same 14 oxides
26.77,21,37.8,52,12.5,14,11.15,16.05,27.86,43.95,0,27 partial molar volumes
"SiO[2]", "TiO[2]", "Al[2]O[3]", "Fe[2]O[3]", "FeO", "MnO", "MgO", "CaO", "Na[2]O"
"K[2]O", "P[2]O[5]", "NiO", "Cr[2]O[3]", "H[2]O+", "H[2]O-", "CO[2]", "SO[2]"
Si,Ti,Al,Fe,Fe,Mn,Mg,Ca,Na,K,P,Ni,Cr,H,H,C,S
4674,5995,5292,6994,7773,7745,6028,6901,7418,8301,4362,7858,6842,1111,1111
2727,5005      # to convert oxides to %
AN,Q,or,ab,an,lc,ne,kal,C,di,hy,wo,ol
ac,mt,il,hem,ti,ap,cc,pero,wus,ru,KMS,NMS,COS      CIPW names
-2.15,0,-8.35,0,-4.5,0,-5.44,.07,3.54,4.19,0,0,0,0      Sack et al. data
40  the 40 names below are used by Igpets to convert say ba to Ba or RB to Rb.
You can add to this list but you must change the 40 to the new sum.
{87}Sr/{86}Sr,{143}Nd/{144}Nd,{206}Pb/{204}Pb,{207}Pb/{204}Pb,{208}Pb/{204}Pb
{10}Be,Be,Li,"H[2]O+","H[2]O-"
Rb,Ba,Sr,Cr,Ni,Cu,Zr,Hf,Nb,Ta
La,Ce,Pr,Nd,Sm,Eu,Gd,Tb,Dy,Ho
Er,Tm,Yb,Cs,Th,Pb,Co,Zn,Sc,Ga
```

DEFAULT.NRM normalization used in S-Norm in variable calculator, set the file you want in the preferences window

```
'Sun and McDonough 1989  primitive mantle
Cs,.0079
Tl,.005
Rb,.635
Ba,6.989
W,.02
Etc.
```

PAGE.DIA controls where Igpets draws its plots on a page there are 16 options.

```
8500,11000,"page width, height in Portrait mode in 1000's of 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"
```

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 1000's 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.DIA This file controls spider diagrams.

```

"REEs-Nakamura, 1974",Chondrites      'title, normalization factor
15,x,1,1000                          '# of elements, no double norm, ystart, yend
La,Ce,Pr,Nd,Pm,Sm,Eu,Gd,Tb,Dy,Ho,Er,Tm,Yb,Lu
.33,.865,.112,.63,1,.203,.077,.276,.047,.343,.07,.225,.03,.22,.034
"Thompson, R.N., 1982-double","Chondrites"
19, "Yb=10",1,1000                  'double norm. to Yb=10, " "s needed
Ba,Rb,Th,K,Nb,Ta,La,Ce,Sr,Nd,P,Sm,Zr,Hf,Ti,Tb,Y,Tm,Yb
6.9,.35,.042,120,.35,.02,.328,.865,11.8,.63,46,.203,6.84,.2,620,.052,2,.034,
"Mg-norm Minors & Majors"," CI (A&G)"
13,"Mg=1",.001,10                  'double norm. to Mg= 1, " "s needed
Ca, Al, Ti, Mg, Si, Cr, Mn, K, Na, Fe, Ni, P, S
9280,8680,0436,98900,106400,2660,1990,0558,5000,190400,11000,1220,62450
"Wood, D.A. et al., 1979","Primordial Mantle"
19,x,1,1000
Cs,Rb,Ba,Th,U,K,Ta,Nb,La,Ce,Sr,Nd,P,Hf,Zr,Sm,Ti,Tb,Y
.019,.86,7.56,.096,.027,252,.043,.62,.71,1.9,23,1.29,90.4,.35,11,.385
1527,.099,4.87
"Sun (1980)","Chondrites"
16,x,1,1000
Rb,Ba,Th,U,Nb,Ta,K,La,Ce,Sr,Nd,Sm,Zr,Ti,Gd,Y
.35,3.8,.05,.013,.35,.02,120,.315,.813,11,.597,.192,5.6,620,.28,2
"Pearce, 1983","MORB"
15,x,.1,100
Sr,K,Rb,Ba,Th,Ta,Nb,Ce,P,Zr,Hf,Sm,Ti,Y,Yb
120,1245,2,20,.2,.18,3.5,10,534,90,2.4,3.3,8992,30,3.4
"Hickey/Frey 1986","Bulk Earth"
15,x,1,1000
Cs,Rb,Ba,Th,K,Nb,La,Ce,Sr,Nd,Zr,Sm,Ti,Y,Yb
.012,.35,3.5,.042,120,.39,.31,.81,11,.602,5.6,.196,620,2.2,.21
"Sun/McDon. 1989-PM","Primitive Mantle"
22,x,1,1000
Cs,Rb,Ba,Th,U,Nb,K,La,Ce,Pb,Pr,Sr,P,Nd,Zr,Sm,Eu,Ti,Dy,Y,Yb,Lu
.0079,.635,6.989,.085,.021,.713,250,.687,1.775,.071,.276,21.1,95,1.354,11.2,.4
44,.168,1300,.737,4.55,.493,.074
"Semark Chond.", "CI"
9,"Si=1",.02,10                    'double norm to Si=1, " "s needed
Ca, Al, Ti, Mg, Si, Cr, Mn, Na, K
14100,15900,0700,159200,222500,3400,2200,7400,0600

```

*.DGM files

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

"AFM","Irv.+Baragar 1971","thol vs calc-alk"	'name, source, remark or note
"TRI"	'a triangular diagram
"Alk",Na2O,1,K2O,1,END	'see *** below
"FeO*",FeO,1,Fe2O3,.8999,END	'see *** below
"MgO",MgO,1,END	'see *** below
0,1,0,1,0,1	'xmin,xmax,ymin,ymax,zmin,zmax
25	'# of points defining fields
0.686,0.294,1	'x,y,pen (1=pen down 0=pen up)
0.646,0.314,1	etc
0.593,0.347,1,0.534,0.386,1	etc
.....	
2	'# of labels
.7,.15,"Calc-Alkaline"	'x,y, label-1
.3,.6,"Tholeiitic"	'x,y, label-2

*** The three lines that define the parameters begin with the variables name, followed by each oxide or element name and its coefficient. The parameter is terminated with END.
Thus "Alk" = Na2O+K2O "FeO*" = FeO+.8999*Fe2O3.

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 capitals basis with { , }, [,] stripped out.

The following example shows how to accommodate division (A/B).

"%An-Al2O3","Irv.+Baragar 1971","thol-calc-alk"	'name, source, remark or note
"XY"	'an XY diagram
"AN"	'variable name - AN
an,100	'part one of x-variable (100*an)
"/" <i>'if / (or *) appears rather than a field name,</i>	then divide (multiply) part one by part two
an,1,ab,1,ne,.6,END	'part two of x-variable (an+ab+.6*ne)
"Al[2]O[3]",Al2O3,1,END	'y-variable, (name, oxide, coeff.,end)
0,100,40,10,10	'x-axis is linear(0), from 100 to 40
	'tick interval of 10, labels every 10
0,10,25,1,5	'y-axis{linear,begin,end,tickstep, labelstep}
7	'# of points defining fields
40.,15.2 ,1,50.,16. ,1 ,60.,16.8,1, 70.,17.6,1	
80.,18.4 ,1,90.,19.2,1,100.,20.0,1	

The following example allows you to draw a box shape and use a log scale for x and y.

"Y+Nb vs Rb", "Pearce et al. 84", "tectonic"	'name, source, remark or note
"XY Box"	'special form of XY, a Box
"Y+Nb", Y, 1, Nb, 1, END	'defines x
"Rb", Rb, 1, END	'defines y
1, 2, 2000, 0, 0	'x-axis 1=logscale, from 2 to 2000, 0, 0
1, 1, 2000, 0, 0	'y-axis {scale, begin, end, dummy, dummy}
7	'7 x,y, pen points to plot lines with
2, 80, 0, 55, 300, 1, 400, 2000, 1, 55, 300, 0, 50, 1, 1, 51.5, 8, 0, 2000, 400, 1	
4	'4 interior labels
5, 750, "syn-COLG", 300, 600, WPG, 6, 3, VAG, 300, 8, ORG	

*.CMA files

The format of these files is almost the same as that for the DGM triangular files. There are three added data, the final apex scaling values. These numbers follow the apex names. They can be in molar, weight or oxygen units.

"Plag. Proj.", "Baker and Eggler", "mole"	'name, remark or note, units
"TRI"	'a triangular plot
Ol, 1	'left apex name, scaling value (1 -mole units)
Al2O3, .5, Fe2O3, -.5, FeO, .5, MnO, .5, MgO	
.5, CaO, -.5, Na2O, -.5, K2O, -.5, end	'the equation
Di, 1	'top apex, etc
Al2O3, -1, CaO, 1, Na2O, 1, K2O, 1, end	'equation for top apex
"Qz+Or", 1	'right apex, etc
SiO2, 1, Al2O3, -.5, Fe2O3, .5, FeO, -.5, MnO	
-.5, MgO, -.5, CaO, -1.5, Na2O, -5.5, K2O, -3.5, end	
0, 1, 0, 1, 0, 1	'xmin, xmax, ymin, ymax. xmin, xmax -a full triangle
0, 1	'no interior lines, '1 extra label
.5, -.07, "Opx"	'extra label
"Di to En-Pl-Q", "Merz.+Eggler", "mole"	'second example
"TRI"	
"En-50", 1	
Al2O3, 1, Fe2O3, -1, FeO, 1, MnO, 1, MgO, 1, CaO, -1, Na2O, -1, K2O, -1, end	
"Pl-60", 1	
Al2O3, 1, Na2O, 1, K2O, -1, end	
"Q+Or-90", 1	
SiO2, 1, Al2O3, -1, Fe2O3, 1, FeO, -1, MnO, -1, MgO, -1, CaO, -1, Na2O, -5, K2O, -3, end	
0, .5, .1, .6, .4, .9	'only a small part of triangle is drawn
0, 0	

***.CMA files continued**

```
                                'third example
"Plag. Proj.", "Grove etal 84; Sack etal 87", "Oxygens"
"TRI"
Ol,4                                '4 Oxygens for Ol
TiO2,-1,Al2O3,.5,Fe2O3,1,FeO,.5,MgO,.5,CaO
-.5,Na2O,-.5,K2O,-.5,Cr2O3,-.5,end
Di,6                                '6 Oxygens for Di
Al2O3,-1,CaO,1,Na2O,1,K2O,1,end
Q,2                                '2 Oxygens for Q
SiO2,1,TiO2,1,Al2O3,-.5,Fe2O3,-1,FeO,-.5,MgO
-.5,CaO,-1.5,Na2O,-5.5,K2O,-5.5,Cr2O3,.5,end
0,1,0,1,0,1
22                                '22 line segments drawn
.29,.71,0,.29,.58,1,.285,.43,1,.285,.39,1,.275,.325,1,.25,.27,1,.26,.2,1
.27,.09,1,.27,0,1,.146,0,0,.165,.065,1,.21,.18,1,.25,.27,1,.08,0,0,.10,.09,1
.12,.17,1,.14,.24,1,.16,.3,1,.19,.36,1,.22,.40,1,.25,.42,1,.285,.43,1
0                                'no extra labels
```

EXTRA.DIA

Parameters that are automatically calculated and added to the variable list when the file operations, extra menu is selected. Also calculated in this routine is density, after Bottinga and Weill (1970) on a water-free, 1 atm, 1200 C basis.

```
"FeO*"                            'name
FeO,1,Fe2O3,.8998,end            'FeO*=FeO+.8998*Fe2O3
"Mg#"                            'name
MgO,2.481,"/"                   'part1 is 100*MgO/40.32
MgO,.0248,FeO,.013918,Fe2O3,.012523,end
                                'part 2 is MgO/40.32 + FeO/ 71.85 +2*Fe2O3/159.7
                                'end signifies the end of the equation
```

PEARCE.DIA

Pearce diagrams are based on element proportions, E.

$E = (\text{wt\%} * \# \text{ of cations}) / \text{molecular wt.}$

These are calculated for all the oxides in the Pearce subroutine. The data file consists of meaningful combinations of these element proportions. Consult Stanley and Russell (1989) for the appropriate use of these parameters.

```
"K", K2O,1,end          'K=K2O , a conserved constituent.
"Ti", TiO2,1,end         'label, oxide, coefficient
"Si", SiO2,1,end
"Al", Al2O3,1,end
"0.5(Mg+Fe)", FeO,.5, MgO,.5,end
"OL+CPX+PL", CaO,1.5, Al2O3,.25, FeO,.5, MgO,.5, Na2O,2.75,end
"Ca+0.5(Na-Al)", CaO,1, Na2O,.5, Al2O3,-.5,end
```

MINS.DIA

This file sets up a few mineral plots. The first plot is elaborate and must always be the first plot in MINS.DIA. This is the geothermometer of Lindsley and Anderson (1983).

Some complicated logic is built into IGPET to calculate this and the logic depends on this plot being the first mineral plot. The other mineral plots are rather plebeian. The Lindsley Anderson geothermometer lacks calculation subroutines for OPX and PIG.

```
"Lindsley-Anderson isotherms"    Title
"CPX", "CPX"                      plots only Cpx
"TRI"
"En", MgO,1,END                   'X
"Wo50", CaO,1,END                 'Y
"Fs", FeO,1, MnO,1,END            'Z
0,1,0,.5,0,1                     'xmin,xmax,ymin,ymax,zmin,zmax
62                                '# of points defining fields
.510,.490,0,.489,.481,1
.458,.472,1,.431,.469,1
.389,.461,1,.341,.459,1.....    'first 6 points
2                                  'two labels
.5,.3,"1200 C"                    'label 1
.37,.345,"1000 C"                'label 2
```

***.PCS files**

These files are control files for MIXING.EXE. They have the partition coefficient data. Values shown here are from Gill (1981).

Note: Tab delimited data so easily read and manipulated in Excel.

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

***.MWT files**

These files are control files for MIXING.EXE. They have the weighting scheme for the oxides.

```
SiO2","TiO2","Al2O3","FeO","MnO","MgO","CaO","Na2O","K2O","P2O5","NiO","Cr2O3"  
.4,1,.5,1,1,1,1,1,1,1,1,1
```


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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