Igpet for Mac

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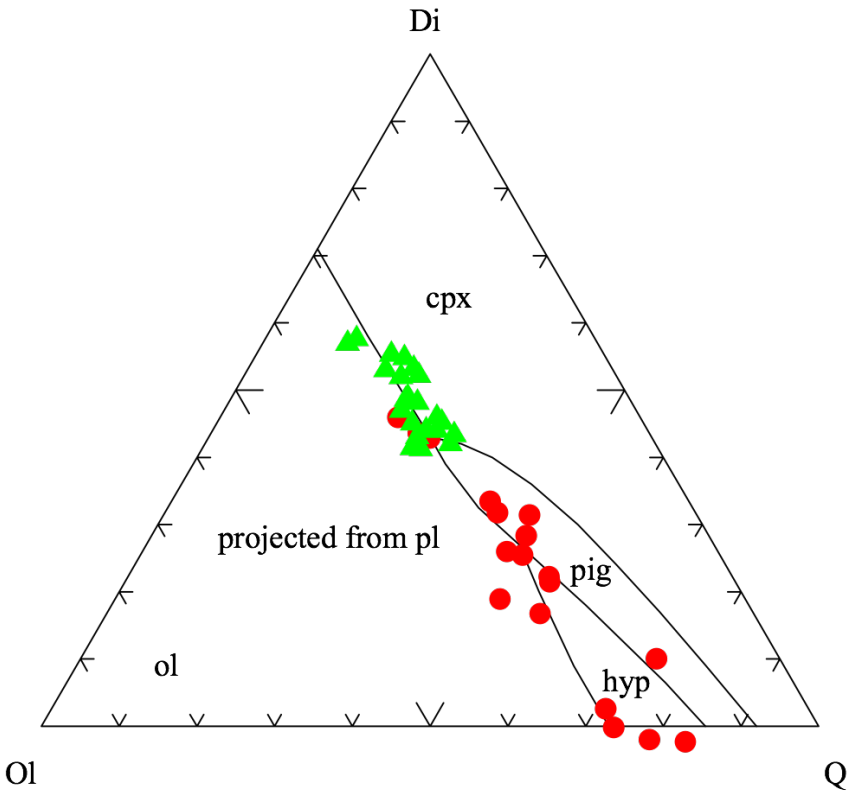

1 atm pseudo-ternary cotectics

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

24 February 2017 Changed file structure to make Igpet work in OSX Sierra. Code Signing was added in December, so installation on Sierra should be OK.

6 January 2017 Changed "Scale to Variable" to adjust sizes of symbols

29 December 2016 Modified PDF setup, added Installation help

6 April 2016 Improved Spider modeling by calculating and displaying the maximum % of melting for non-modal melting. Made PageMax automatic if Position is anything other than default.

15 March 2015 Changing colors in the Symbols page resulted in new colors on the screen but the new colors were not carried over to the PDF version, which is the only version that can be saved. At least the repair was easy.

Nov 25, 2015 Many small improvements based on experience in creating the Igpet Work-book. Clarified the use of several Diagram files: IrvineBaragar.txt, DiscrimBasalt.txt and RockType.txt. Posted Igpet Workbook to homepage. Created a Teaching version of Igpet.

Sept 23, 2015 Fixed missing isotope calcs for spider mixing, (Pb isos)

August 24 2015 Added new PC file from Laubier et al. 2014. Added Tormey et al. (1987) and Grove et al. (2003) and improved other CMAS projections from Grove's research group.

August 21 2015 Once again repaired Igpet's ability to read data files in formats other than US English. Nthfield() was adding quote marks if a , was the decimal marker.

May 16 2015 Minor change in calculation of eNd_o in extra.txt. Made the value of CHUR visible and added a o subscript to indicate that this is a zero age calculation.

Jan 22,24 2015 Repaired flaw in trace element calculation in Mixing. Flaw was introduced in December. In Igpet, made the launch of Preview optional when saving a diagram.

Jan 12 2015 Adobe Illustrator was translating the x-axis numbers into a continuous string, making it awkward to edit in Ai. Fixed this by adding dummy print commands. Now each label is discrete. Fixed in XY, Spider and Histogram plots.

Dec 10-14 2014 Added ability to draw double triangles "DTRI" for IUGS rock classification and allowed small fonts in PDF Diagrams. Simplified the calculation of normalized element values Eu* etc. Changed output logic for Mixing, CIPW and PTfO2. Fixed a bug in Igpet's 'add a file' logic.

Nov 20, 2014 Added logic that allows a Legend to be plotted for a histogram.
Made major internal changes to file handling and plotting of characters on the screen. These changes were required to accommodate the phasing out of useful functions in the XoJo programing language. They "should" be invisible to users. Rewrote and simplified the isotopic mixing in SpiMix using DePaolo equations. This allows mixing for epsilon Nd and epsilon Sr. Removed a glitch for mixing and modeling Pb isotopes in spiderplots. Created a Teaching version of Igpet that writes jpeg files.

June 30, 2014 Added polynomial regression to XY plots

Feb 8, 2014 Repaired a bug in File Operations-Add a file

Nov 24, 2013 Created a utility to partition Fe3 and Fe2 using Beattie (1993) and Kress and Carmichael (1991). Incorporated this logic into Igpet for CMAS and Pearce calculations, replacing the Sack et al (1980) logic that used just one T and fO_2

Nov 10, 2013 Created a Zoom button to blow up a portion of an XY plot. It is a crude zoom that needs to be adjusted with an Axis call.

Created decent Mineral plots for Feldspars and the PX quad. Made the mineral keys the same on all PC files added another special keyword, "Mineral" to identify the minerals in mineral data files, e.g. ol is olivine. Significant changes in Mixing program and Mineral Plots to use this new keyword.

Aug 22, 2013 Added Hoffman (2007) Mantle isotopic diagrams

Aug 4-8, 2013 Added ability to read csv (comma delimited) files and the ability to convert many GEOROC column headings (variable names) to Igpet friendly names. Made the file read method identify the first occurrence of "samp" in the top row as the column of sample names. Made several other small improvements.

June 13, 2013 Major upgrade to vector graphics as PDF function is added. No doubt many bugs are crawling about but still a huge improvement in output quality

June 6, 2013 Refixed the Axis bug of March 25 and extended the fix to other areas that use inputfrm.

May 29, 2013 Changes some logic in Spider plots to allow spaces to be ignored in element labels in spider.txt

March 25 2013 Fixed Axis bug introduced by REALbasic change

Feb 21, 2013 Fixed flaw in Lindsley Anderson px geothermometer, now correct again.

Jan 3, 2013 Fixed flaw in mixing if the variable was [N] normalized (S-Norm function)

Oct 2, 2012 substantial improvement of REE Inverse modeling

Aug 29, 2012 Added mixing and recharge models to Spider modeling. Made new PC files. Added Mantle_traces data file.

Aug 15, 2012 Cleaned up some issues in XY Models. Improved the Variable form

Aug 7, 2012 Added ability to use epsilon Nd and epsilon Sr in AFC models in Spider plots.

May 16, 2012 Fixed various flaws in histogram, principally concerning Log values. Added logic to allow user to change the suggested % melts for Spider modeling. File PercentFs.txt holds the strings of melt %s .

Apr 19, 2012 Found and fixed a serious flaw in the AFC calculations for isotopes in the Spider modeling section.

Oct 16, 2011 Added a legend that writes a separate diagram, just a legend.

Dec 17, 2010 Fixed a flaw in Equilib. Xtall. Calculation in spider modeling. Made changes to Histogram but still have some uncertainty about the correctness, so I will revisit it.

Aug 31 2010 Minor changes to ferrous ferric ratio adjustment

Jan 2010 Improvement to $C_oD_oP_i$, REE inverse modeling**.**

Aug 26, 2009 Series of significant changes. Added more diagrams and the 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 calculations 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 ",".

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, Esteban Gazel, Fara Lindsay 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 Igpet improves.

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Graphical Aids for Interpreting Geochemical-Petrological Data: Peaks & Pitfalls

Igpet and Mixing can display data beautifully and make a variety of complicated calculations, but rarely do these tools prove anything! What these programs can most reliably do is prove hypotheses incorrect. Usually, after considerable effort, one can find a version of a hypothesis, such as fractional crystallization, that is consistent with available evidence, not that it is proved. All too often this inherent limitation is forgotten and weak hypotheses are deemed correct 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 as well as some helpful approaches.

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 cooperative. 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 first hypothesis to test.

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 likely 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 in a large magma chamber.

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, although 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: Using geochemical data: Evaluation, presentation, interpretation.

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 a mixing line between end-member compositions, but all the detail concerning the relationships among the actual samples becomes highly compressed. Furthermore, 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 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 available in Igpet judiciously. Few of the volcanoes I have looked at are homogenous. In my experience, 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. 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 the subdividing and then back off and combine similar groups. At the other extreme, some geochemists never subdivide at all.

Obviously, these remarks prove that 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 al. (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 depleted mantle (DM) 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, a lower carbonate ooze and an upper hemipelagic mud. 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. Y, like the HREE, 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 with its many subsets). I highly recommend this. It is remarkable how different arc geochemistry can be given the similarity of process. To me, each convergent margin simply has different widows that are open, depending on source differences and process variations.

Using Igpet for Petrogenetic Modeling

(Work through pages 1-10 below before trying the ideas just below)

Igpet has evolved from roughly 1972 to the present. A major consequence is that some parts are more powerful than others and a fair amount of redundancy is present. To most effectively use Igpet I suggest the following approaches for the purposes listed.

Teaching partial melting, mixing (assimilation) and fractional crystallization

Trace element behavior offers useful constraints on the magmatic processes that cause differentiation. Differentiation is the general term for all the processes that cause magma compositions to be different from the solid they melted from or to be different from the parental magma they evolved from. Melting, magma mixing, assimilation and crystallization differentiation are the primary processes. Modeling trace element behavior requires some decent starting compositions (typically mantle compositions or parental magmas) and knowledge of Kds (Nernst distribution coefficients) or, more generally, partition coefficients.

$$Kd = \text{concentration in mineral} / \text{concentration in melt}$$

The bulk partition coefficient, D, is the weighted sum of the contributions of all the minerals in equilibrium with the melt.

$D = \sum x_i * Kd_i$ for i=1 to n minerals. The x_i values are the mineral proportions (they must sum to 1)

For a given element, the Kds for different minerals vary strongly with magma composition, mineral composition, T, P, fO_2, water content and other factors. Some Kds are primarily temperature dependent, others have stronger variation with pressure. Because there are multiple causes of Kd variation, there is no, fixed best set of Kds.

With that super brief introduction, the trace element modeling process in Igpet is:

1. select a starting composition (Igpet has a file called Mantle_traces.txt for melt modeling)
2. select a model such as batch melting, fractional crystallization, mixing etc.
3a. determine the mineral mode: the minerals and their x_i values or proportions.
3b. determine the melt mode (proportions of minerals entering the melt.)
4. select a file of partition coefficients appropriate for the composition, temperature, pressure, fO_2 etc of the system you desire to model.
5. calculate Ds (and Ps if needed) for each element of interest using the data in steps 3 and 4.
6. for a range of F values, usually % liquids or % melts but also mass ratios in some AFC models, use the selected model's equation to determine the values of each element at each value of F.

In the Spider diagram-Model option Igpet does all these steps and plots the results on the spider diagram you are using. The eventual goal is to get to this stage of complexity, so that you can test various models with some rigor. However, this is complex and the result, a spider diagram where small and moderate scale variations in element behavior get lost in the $\log_{10}$ scale of the Y-axis, is opaque to most new petrology students.

Therefore, I suggest starting with the XY-Model option. Igpet has primitive modeling tools here. In the XY-Model, Igpet combines steps 3, 4 and 5 and simply asks you to supply a D value for each element. Igpet suggests a range of F values and then graphs the result. This is immediate and interactive and should readily show how differently elements behave depending on D values. The cases of D=1, D<1 and D>1 yield very different element behavior.

Start with the Boqueron.txt data file and plot SiO_2 versus K_2O. Click **Model** and ***FC*** (Fractional Crystallization). Reasonable D values are 0.78 for SiO_2 and 0 for K_2O. Use sample B6 as the parent or Co.

Sr can have D values from 0 to 2, depending on how much plagioclase is present. Plots of Sr versus Ba or K will be useful for a well-behaved data set. With the Boqueron file a plot of MgO versus Sr reveals a two-stage evolution: first from B6 to B2 and second from B2 to B3. Plot K_2O versus Sr and then use trial and error to find appropriate D values for the two stages of magma evolution. Sample B2 is the most evolved sample without removal of plagioclase, after B2 (i.e. at lower MgO than B2) plagioclase is being removed and Sr decreases. This data set is unlikely to be the result of simple two-stage fractional crystallization because the first stage needs a D of about 0.6 for K, quite a bit too high. The second stage has a D of about 1.8 for Sr. This also is quite high.

Now select a data file with a mantle composition or two and a comprehensive set of trace elements and isotope ratios. CAVF.txt is such a file and will allow you to explore some equilibrium melt examples and a few examples of ratio/ratio plots (e.g. 1/Sr versus Sr isotopes) or Ce/Pb versus La/Yb. Near the bottom of the CAVF sample list are two model mantle compositions, the first, from Utila Island off the Caribbean coast of Honduras, has a relatively flat pattern, and the second, DM_SO_Nic, has a depleted Morb signature. These mantle compositions can be used to model batch melting. Use ***Equi. Melt.*** and assume all the melt is extracted at a particular degree of melting. The XY Model tools have only the one melting option, modal batch melting. Try modeling Ce/Pb versus Ba/La starting from the two local mantle compositions

The next stage is to look at a range of partition coefficients for the same mineral. Depending on the compositions and the conditions of the experiment, there are substantial ranges for published Kd values. The file PlotPCs.txt in the Data Files folder allows one to examine a variety of Kd or partition coefficient values. To use this, first read the file and then **Plot-Spider**. Select ***REEs set to 1***. Adjust the **Y-scale** to Log vales of 0.0001 and 10. Use the **ID ON** button to explore the shapes of the REE partition coefficients for different minerals. Use

Repick to reduce the clutter and see just the garnets (gt) or clinopyroxenes (cpx) or whatever. Note the range for each mineral and the fact that the Y-scale is a Log_{10} scale. Develop a large degree of caution when using PCs.

The extended REE diagram, which includes many LIL elements and HFS elements, is called ***PM set to 1.*** Use **New Spi** and select ***PM set to 1*** to look at the wide ranges of Kds determined for the incompatible elements outside the well-behaved REE group (the lanthanides: Lanthanum, Cerium, Praseodymium, Neodymium, [Promethium does not occur naturally on earth], Samarium, Europium, Gadolinium, Terbium, Dysprosium, Holmium, Erbium, Thulium, Ytterbium, Lutetium, plus Scandium, Yttrium.). Although the extended spiderplots with LILEs (large ionic radius lithophiles K, Rb, Cs, Sr, Ba, Pb and Eu^{+2}) HFSEs (high field strength Ti, Nb, Ta, Zr, Hf, Th, U, P, Ce^{+4}) allow examination of a wider range of trace element behavior, the partition coefficient data are considerably more scattered.

Although the Kd variation is discouraging, there are some reference points worth knowing, especially if your primary interest is the partitioning of trace elements during melting in the mantle. In this case the minerals are olivine, orthopyroxene, clinopyroxene, garnet or spinel and possibly hornblende and a few accessory minerals. To simplify the problem, note first, that Kds below 0.001 are not all that different in their effects on melting as long as the % melt is 5% or more. Furthermore, a mineral with a moderate level of incompatibility (e.g. cpx) will have a dominant effect on the D value and prevent D from being extremely low. Finally, ol, opx, cpx, and gar have similar patterns, regardless of the data source. This is most obvious for the REE, garnet has Kds >1 for the heavy REE, giving a pattern that slopes steeply up to the right. Amphibole has a shape similar to garnet but at lower values. Clinopyroxene has a bow shaped pattern with a maximum in the middle REEs that gets close to 1 but remains beneath 1. Olivine and orthopyroxene are low and flat. Spinel is low and flat except for Nb and Ta. When these minerals are present in the residue of partial melting, they impart their signature on the melts. Assuming an initial flat pattern in the mantle prior to melting, the melts generated inherit a trace element signature that is inverse to the shape of the residual minerals.

At this point, consult a petrology or geochemistry text to examine the equations for batch melting, incremental melting, aggregated fractional melting, Raleigh fractional crystallization, magma mixing etc and their derivation and behavior. In particular, carefully review plots of F, amount of fluid or liquid, versus C_l, concentration in the liquid. Generally, the initial concentration C_o is taken as 1 and curves are drawn for different values of the bulk distribution coefficient, D. If D is extremely low (a harzburgite residue, for example), then small values of F result in huge enrichments of elements with very small D, so small degrees of partial melt can change the ratios of highly incompatible elements, D=0.001 compared with incompatible elements D=0.01. In contrast, fractional crystallization causes negligible separation of these incompatible elements.

An unknown that Igpet cannot help you with is the modal composition of the mantle. For a peridotite mantle there is, of course, a high proportion of olivine. The mode of minerals in

the mantle depends on the mantle brought into a melt condition at the various tectonic settings that generate melts; e.g. MOR, oceanic island, arc etc. In addition to the mantle mode, a melt mode is needed because one cannot expect the minerals in the mantle to enter the melt in their pre-melt proportions. This is called non-modal melting (Shaw, 1970). It is the realistic case where minerals enter the melt in proportions controlled by phase relations that vary with X_i, T and P. In choosing a melt mode there is flexibility but pay attention to the experimentally determined phase relationships. The aluminous mineral present varies from plagioclase at quite shallow depths, e.g. below 1 GPA or 35 km, to spinel and then to garnet at about 2 GPA or about 70 km.

Now make melt models using the **Spider-model** tool. Mantle_traces.txt has 4 mantle compositions, two non-depleted (flat) patterns and two depleted choices, with much lower values for the more incompatible elements to the left hand side of the diagram. Pick a spider-diagram like McDon. & Sun 95 and select all the mantle models. Adjust the **Axis** and use the **ID ON** function to see which is which. Use **Repick** to select a particular mantle source. Now press the **Model** button and select **batch melt** or **agg fract melt.** Aggregated fractional melting is likely the most realistic physical model of melting. It is worthwhile comparing agg fract melt and the computationally simpler batch melting.

For non-modal melting Igpet needs two mineral assemblages, one for d and another for p.

Batch melting equation: derived from mass balance constraint.

$$C_l = C_o / [d + f * (1 - p)]$$

Aggregated fractional melting equation: See Albarede (1995) for derivation

$$C_l = C_o * [1 - (1 - f * p / d) ^ (1 / p)] / f$$

*Aside: the term (1 - f * p / d) can be negative for p much larger than d. Igpet assumes that 1/p is not an integer and therefore inserts a blank for C_l in such cases. There are similar checks for illegal function calls in several of the spider models. If some of your spider models mysteriously lack an element or two at some F value, this is the likely reason.*

Having selected a model (batch or aggregated melting), you now need to fill in the blanks on the spider model window, before clicking the Calculate button. Start at the top and work down: PC file, Source, Mantle mode and Mineral mode. At this point Igpet calculates the maximum % melt possible for the mantle and melt mineral assemblages chosen. Keeping the maximum in mind, adjust the suggested melt percentages as needed.

I suggest using the Salters and Strake DMM as your starting mantle and the PC file at 3 GPA by the same authors. Make a model using the non-modal agg fract melt option and then make a second model keeping everything the same but selecting batch melting. How different are the two sets of models? Having compared the models on the spider diagram, now **Plot XY** and compare La/Yb versus Ba/Nb or Ba versus Sr or whatever.

The power of the Spider model option comes from two features. First, Igpet keeps the calculations in memory and allows you to evaluate the models in greater detail using X-Y

plots, which are much more sensitive than the log based spider plots. If all the required data are present (e.g. ppm Sr and the isotopic ratio), Igpet will calculate the isotopic ratios and the epsilon Sr and epsilon Nd for different models. For melting, this is trivial: just give the melt model the same isotopic ratio as the mantle source. For more complicated problems, such as mixing and assimilation or AFC, Igpet's ability to calculate isotopic variations is quite useful because isotopic constraints are stronger than trace element constraints.
The second powerful aspect of Spider models is the simultaneous modeling of multiple elements. The elements that are modeled are the ones found in the PC file and also in the data file. The list of elements in the spider-diagram is not used in the modeling. Therefore, the models may fail to include elements in the spider diagrams, but may include other elements that are not in the diagram. It is important to carefully examine the PC files because they are the primary control of what elements are modeled.

Forward models
Most modeling in igneous geochemistry is forward modeling. This type of model allows one to assert that a particular hypothesis is allowed. This is a weak constraint but a surprising number of hypotheses can be ruled out by numerical tests of forward models.

Create an appropriate mantle
If you have an aphyric lava with a high MgO content you can estimate the mantle it came from using spider modeling and choosing the **Inverse option**. You need a PC file for the incompatible elements of interest and mineral modes for the mantle and the melt. Given all the error that the weak constraints allow, it might be advisable to use modal batch melting. Picking the "best" F is difficult, especially for alkaline lavas for which F is likely to be quite small. However, the goal is to create a plausible model not perfection. The local mantle you "create" should have the same general spider diagram shape as a more generic global mantle type such as DMM (depleted MORB mantle) or OIB (ocean island basalt) mantle or pyrolite mantle. Creating your own starting source composition allows local trace element variations to be incorporated at the beginning of the modeling process. A separate approach, perhaps appropriate for a batch of lavas from an oceanic island, is a blended mantle. Many OIBs seem derived from a mixture of deep plume mantle and shallow asthenospheric mantle. Under continents one can also mix in some lithospheric mantle. If your lava series appears to be a mix of identifiable mantle components, you can create a blend of components in the spider diagram using the **Mix** button.

Create a suite of parental magmas
Actual parental magmas are very rare and difficult to prove. However, in a model you can specify your assumptions and create a range of parental magmas. If your lava suite has a large range of incompatible element contents for a small range of MgO, then you likely have a collection of melts of the same (highly similar) mantle that formed by different degrees of melting. Alternatively, you may have sampled many small volumes of mantle that were enriched/depleted to varying degrees but melted to the same extent. Ideally, the latter case should have strong isotopic variations whereas the former case will have no isotopic variation. You can also have two distinct mantles (one a predominant composition, the other a

set of veins in the predominant composition). Unfortunately, the possibilities keep expanding. If you have well behaved samples and high quality isotopic and trace element data, you should be able to weed out some of the ideas.

Try simple models at first and create a petrogenetic grid, a set of possible parental magmas generated by different F values and changes in the mineral mode. For example, including more or less garnet has strong effects and is a plausible cause of HREE variation.

Many cases will not require a grid because your lava series is simply one large melt batch that differentiated to some degree in the near surface environment.

Fractional crystallization

Most or all of your lavas likely have lower MgO than your modeled parents. Use fractional crystallization (using the minerals found in the more mafic lavas) and low pressure partition coefficients to see if fractional crystallization models that start from your calculated parental magmas can reproduce your evolved lavas. If so, then you have a consistent story.

Assimilation Fractional Crystallization

It is likely that your evolved magmas interacted with the crust they passed through. If so, you need samples of wall rock to define an appropriate contaminant. Isotopic data are very important for selecting an appropriate contaminant. Now select an appropriate parental magma and a contaminant and see if you can explain your data array using AFC. Read DePaolo's paper to understand the r parameter and some of the non-intuitive results AFC can lead to. This is a powerful tool but I recommend keeping the r values close to 1.

REE Inverse Model

Inverse modeling provides a stronger constraint that forward modeling and ideally can define a limited field of allowable conditions from a minimum of prior assumptions. Igpet incorporates the incompatible trace element inverse model built by Feigenson and Hoffman. It is the C_oD_oP model in Spider modeling. See Feigenson et al. (1996) for a comprehensive description.

Why Igpet?

The power of Igpet is that you can make many models very quickly. By incremental change or trial and error it is often possible to arrive at a comprehensive set of assumptions about sources and processes that allow you to reproduce your data array. Thus you have a plausible story. It is not easy to make a successful forward model so you have accomplished something useful in doing so. Unfortunately, a successful forward model is only a possibility not a proof. It would be useful to create a successful forward model and then start again from scratch and go in other directions to see if you can create a substantially different yet still successful model.

Install

In OSX Sierra data files and Apps have to separated, so as of Feb 24, 2017, there are now two zip files to download, IgpetApps and IgpetDocs. Unzip these files with a double-click and place them in the locations specified. All the Igpet support subfolders are in IgpetDocs which MUST reside in the Documents folder. The Apps folder, IgpetApps, is most suitably located in the Applications folder. You can make aliases of the applications, Igpet, Mixing, PTfO2 and CIPW for the desktop. The current version of Igpet is called Igpet_Sierra because the Sierra OS required a significant change in file structure. The other apps, Mixing, Cipw and PTfO2 were not affected.

Starting with the 2017 version, the italics section below should no longer be necessary because the apps now are code signed.
Macs have a Gatekeeper that prevents older versions of Igpet apps from running. The workaround is to temporarily change the security setting to "Anywhere." To get to this setting, click the Apple symbol at the top left of the screen, then click System Preferences, then click Security & Privacy. In the window that appears, click on the lock in the lower left, then enter your password. Now modify the "Allow apps downloaded from:" section by clicking the radio button next to "Anywhere." Click the lock again to close it. Exit System Preferences. Now open and run each of the 4 apps in the Igpet folder. Just start each App and then quit.

Finally, reopen System Preferences, return to the security settings and change the "Allow apps downloaded from:" selection to "Mac App Store and identified developers". Close System Preferences and explore Igpet.

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, start Igpet. By doubleclicking the app. The main Igpet window appears. Options can be selected by clicking menu items or buttons.

Read a File

First, click the menus **File**, **Open File**, then use the file dialog box to select a data file with an extension like .TXT or .CSV. 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 the menus **Plot, Histogram** and you will be asked to select the X-axis variable for a histogram using the Variable window, which is a grid of buttons labeled with the file's column names, e.g. SiO2. There is also a primitive calculator and a text box for directly 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 colors of the symbols assigned to 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. To draw a normal curve on the histogram, use 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, such as a histogram. 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 and to the left of the graph allow 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 redrawing the first sample as a black circle. 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 redrawn as a black circle 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 a black circle. 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.

A **Zoom** button asks you to select a lower left point and an upper right point, so you can zoom in to a sub-region of an XY plot. This is a crude tool that needs a subsequent **Axis** call to tidy up.

Add a Legend

The **Legend** button asks you to select a legend file. There is a legend file for the Fusama data, called: LegendFusama.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. **Keep all the Legend files in the Data Files folder. That is the only place they can be seen by Igpet.**

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. In such cases, the computer can help you imagine variation, when, in fact, the spread is just noise.

To change the axes, click the **Axes** button near the top left 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

The **Aspect** button allows you to change the shape of your graph. The default aspect ratio for Igpet is a rectangle, designed for 35mm slides, an obvious anachronism! However, this shape is also suitable for Powerpoint. 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 **Position** button, a choice under **Aspect**. These positions are specified in a file called Page.txt. Using TextEdit, you can modify them to suit your needs. See Appendix A for details. **PageView** lets you see how diagrams fit on a page.

View a third dimension
The **Value** button 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 **Value** 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 **Symbol**.

Click **Refresh** to see the symbols. Eliminate a symbol 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 box adjacent to the open red circle. 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 color dialog. You can explore more pleasing color combinations and save the RGB definitions of the colors by writing them down and later using them to make your own symbol file with a new name like: mysyms.sym.txt.

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 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 independent criteria, such as stratigraphic grouping; petrographic characteristics; TiO_2 concentration, shape of REE pattern, etc.

The **Scale to Variable** radio button allows symbol size to vary with a parameter like MgO or Ba/La. To set the scale, first make a plot with the desired scaling parameter as the X variable. Click the **Symbol** button and then the **Scale to Variable** radio button. Pick the variable to scale to and Igpet suggests scaling factors automatically. Try these by closing the **Symbols** window. If these are not suitable, click **Symbol** again and repeat the process but adjust the scaling factors manually. Moving them closer together gives a larger range of symbol size.

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 some displays. 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.txt, to get greyscale symbols. In the **Symbols** page click **New sym file** to load a new symbol file.

Tie Lines draws tie lines between each successive point, 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 spider-diagrams, 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 because of dithering. If so, use **Black Syms** and the symbol borders will re-appear.

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 and *PowerPoint* created a need for full screen color. These color backgrounds can be transferred to graphics programs, like *Adobe Illustrator*. **Pagecolor** and **Boxcolor** let you set these two areas to any possible color. **Whitepage** and **Defaultcolor** do what their names imply. Now click **OK** and return to the main screen.

Select Subsets of your data

The **Select Subsets** button allows you to filter your data through a huge number of 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, so eliminate them, by clicking on **Select Subsets** and then doubleclick **SiO2** in the leftmost panel. The next panel fills with a list of SiO_2 values. Above the third panel, use the controls to 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, almost immediately, just a few subsets, such as individual volcanoes.

Regression calculations

In X-Y plots, the simplest type of modeling is least squares regression. For example, magma mixing should create a linear array in element-element plots. Igpet uses the algorithms in Davis (1973) for linear regression and the Pearson correlation coefficient. After transformation of variables, the same logic allows polynomial regression and hyperbolic regression. Spearman's rank correlation coefficient was calculated using equations from Swan and Sandilands (1995). Statistical parameters were checked against data and results in Swan and Sandilands (1995).

Click the **Regress button** to select a polynomial regression. There are two choices for linear regression. The old one has more options and statistics: the regression line can be drawn through either the range of X-values or the length of the X-axis, 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). Regression parameters (slope, slope error, intercept, intercept error) can be printed on the diagram or saved to a text file, called stats.txt. Next, you are asked to add the line to the plot or not.

The polynomial choices; linear, quadratic and cubic, draw the equation across the full x-axis and provide Fi statistics, the F for the added term. Using the degrees of freedom (1, n-order), compare Fi to the critical F in a table of F values to determine if the additional polynomial term is warranted.

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 Subsets** 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** buttons uses the equations derived by Langmuir et al. (1977). **Mix** 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. I'm not sure there are any interesting mixing plots for FUSAMA.txt but there are in the file CAVF.txt. These data will allow you to reproduce the diagrams in Carr et al., (1990).

So open CAVF.txt and plot Ba/La versus La/Yb or $^{87}Sr/^{86}Sr$ versus $^{143}Nd/^{144}Nd$.
First, you need to use the identify button (**ID ON**) to choose which samples to use as endpoints. Second, click the **Mix** button and 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.

The **Mix-Least Squares** buttons fit 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 (in X-Y plots)
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.TXT. This file will allow you to reproduce Figure 3 in DePaolo's article and, in the process, learn how this modeling works.

For a simple test of **Model**, reload the FUSAMA.TXT file and plot SiO_2 vs. K_2O. Consider the red symbols for Santa Ana and 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 keep 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 considerably more powerful model option available with spider diagrams.

Error Bars
If a data column is followed by a column headed by “error”, Igpet recognizes the second column as the ± error and plots an error bar. To see how error bars work, read the file Boqueron.txt and plot 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, calculate a Ba/La column and place the propagated error in the next column with the header “error.”

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, **Quad**, 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 a great way to see large variations in incompatible elements at a glance. Because of the log scale you miss the detail seen in XY plots, especially plots of incompatible element ratios. Nevertheless, it is a powerful tool. Unfortunately, there are too many spider-diagrams. The best spider diagrams 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, McDonough and Sun (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 by particular instruments. In Igpet the missing elements show up on the x-axis but no symbol appears (e.g. Pm and Tb). Use **Stagger X** to get a double or single line for the elements on the x-axis.

Repick, **NewSpi** and **Y-Scale** are special buttons for the spider diagrams. To see them, first select **File-Open File** CAVF.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.

Mixing in Spider plots

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. Sr, Nd, Pb, and Hf isotope ratios are also mixed. Logic for eNd, eSr and Os is present but not well tested yet.

Modeling in Spider plots

Elaborate partial melting, crystallization and assimilation-fractional crystallization (AFC) models can be calculated while a spider diagram is plotted. The Spider model option allows one to simultaneously model fifteen or more elements plus isotope ratios of Sr, Nd, Pb, Hf and epsilon values of Nd and Sr. The elements that are modeled are the ones found in the PC file selected in the SPIMOD window and also present in the data file. The models remain in Igpet's memory for subsequent use in X-Y plots of elements and isotope ratios and, if desired, can also be saved to a new file. Spider models require partition coefficient files (*.PC.txt files in the folder called PC), a starting composition, and knowledge of melting models. The book by Francis Albarede, Introduction to Geochemical Modeling, should be read carefully before using any of the melting or crystallization models. 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 $C_oD_oP_i$ option in spider modeling uses a trace

element inversion method developed by Feigenson and Hoffman and used in Feigenson et al. (1996).

The AFC models of DePaolo (1980) 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 first, rather than blindly using the software.

In the Spider AFC models a parameter called ep_Nd is recognized by Igpet as epsilon Nd. Similarly, use ep_Sr for epsilon Sr values. For zero age rocks the Add Extra Parameters function in the File Menu will add eNd_o. Igpet recognizes ep_Nd, eNd_o, and ep_Sr as isotope ratios and uses DePaolo's equations 13b and 15b to calculate AFC models. In the data file, Depaolo.txt, are four samples. The first two allow you to recreate DePaolo's figure 4. The last two allow you to recreate figure 6. One first makes the models in the Spider plot, then makes X-Y plots to reproduce the figures.

To use the **Model** option for melting and assimilation/crystallization processes, start by selecting a model, e.g. Aggregated Fractional Melt, then select whether melting is modal or non-modal (Pi's<> Di's). Then pick a partition coefficient file (a pc.txt file), a mantle mode, a melt mode (if non-modal melting), and a set of % melts. For non-modal melting the maximum % melting possible for the chosen mantle and melt mineral assemblages is shown. Keeping that upper limit in mind, adjust the set of % melts.

You can run a melt model 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 made in the XY plots, these calculated results are now 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. It is always best to save the file using a new name.

Output Options

For the professional version of Igpet, the **PDF save** button creates a pdf file. Igpet suggests a file name that merges the data file name and the diagram axes in a File Save dialog so you can place the file where you want. I suggest creating an IgpetPDF folder on the Desktop because diagrams pile up fast. **The PDF output is high quality graphics suitable for publication.** The diagrams are superior to any others made on a Mac by earlier Igpet versions. There is an option in Preferences that causes *Preview* to launch and display the PDF file that was just saved. In *Preview,* use Edit/Copy to copy your diagram to the Clipboard or Print it. By default this option is off. Diagrams saved to the Clipboard are not always correctly rendered in *Adobe Illustrator,* however Microsoft Office renders the same diagrams correctly. It is better to save a PDF file and then read it using *Adobe Illustrator* or *Inkscape.*

Pasting *Igpet* diagrams directly into *Microsoft Office* is simple and effective. For *Word* it is best to right-click or control-click the diagram and select Format Picture. Next, select Lay-out-Tight. You can then place the picture wherever you want. You will be frustrated if you try to ungroup and *Igpet* diagram in *Office*. As far as I know, it is no longer possible. To fine-tune a diagram, get an excellent illustration program such as *Adobe Illustrator (Ai)* or an open source program like *Inkscape*, which is simpler than *Ai* and appears to be free.

For the teaching version of Igpet, the **JPG save** button creates a jpg file. Igpet suggests a file name that merges the data file name and the diagram axes in a File Save dialog so you can place the file where you want. I suggest creating an IgpetJPG folder on the Desktop because diagrams can pile up fast. There is an option in Preferences that causes *Preview* to launch and display the JPG file that was just saved. While in *Preview*, use Edit/Copy to place your diagram on the Clipboard or use Print to get a hard copy. By default this option is off.

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 there is an option for switching back and forth between colored (**Color)** and white (**White**) background 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 top of the file. Use the *TextEdit* accessory. See section below on symbol files.

Page View and Nrml View
This toggles the view of either a whole page (portrait or landscape) or the normal view of a single graph, which is the Portrait-Upper page position.

Multiple diagrams per page
To make a set of eight Harker (SiO_2 versus oxide or element) or Fenner plots (MgO versus oxide or element) all on the same page, first activate **Page View.** Next click menu **Plot-Diagrams** and select Harker or Fenner. Plot the first diagram and it will show up on the page view in its proper place. Next click the **PDF save** button and pick a file name. Next click the **Add latest diagram to plot** button. Next select the **Next diag** button, then click the **PDF save** button and then the **Add latest diagram to plot** button, etc. When you have plotted all eight figures and added them to the plot, click the **PDF save** button one last time and select **Close/Finish page**.

Preferences

The **Preferences** menu brings up a window that allows you to customize Igpet. Four buttons allow you to specify: the font size, 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 five 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. This

is an old part of Igpet, I suggest using the SubSelect window instead. The second switches the y-axis labels to horizontal or vertical. The third allows you to remove the bounding line from filled symbols, The fourth toggles on or off the background color of the box or triangle where the data plot. The fifth toggles Preview to start (or not) when a diagram is saved.

At the upper right of the preferences window is a textbox for scaling the size of the Igpet window. It is advantageous to scale the size of Igpet to be smaller than your screen, this allows Igpet to be a moveable window. Igpet ships with a default width of 1000. I suggest adjusting this so that the Igpet window does not fill the entire screen.

The changes you make in preferences will not do much unless you save them. Your choices go into igprefini.txt 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.

Examine “What_is_igprefini.txt” in the Controls folder if you wish to change the default settings with a text editor.

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 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). The Norm to 100% routine finds 13 oxides: SiO_2, TiO_2, Al_2O_3, Fe_2O_3, FeO, MnO, MgO, CaO, Na_2O, K_2O, P_2O_5, Cr_2O_3, NiO (the last two are typically converted from ppm values) and multiplies them, just before plotting, by:

100/(sum of oxides), in which Fe_2O_3=0 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, FeOt, 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. Note that FeO* is NOT recognized as one of the 13 oxides and will be ignored by Igpet, causing error. Use only FeO or Fe_2O_3 as column headers for the oxides of Fe.

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 and the trace elements listed in Igpet-data.txt are preceded with * indicating that they will be normalized. To do the same for any other trace elements, double-click the element and an * will be added, telling Igpet to normalize this element. When done, move to Quit at the end or beginning and double-click, or 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 discriptor, 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. The normalization is part of the definition of the diagram.

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 allows one to us the logic of Kress and Carmichael (1991) to reset the Fe oxides. If you chose to reset the Fe oxides, temperature is determined from lava composition following Beattie (1993) and fO_2 is set following a choice of an oxygen buffer. You can also use the utility program, PTfO2.app, to calculate Fe_2O_3 and FeO and use the generated values to replace the Fe oxide values in your data file. I suggest keeping the original data columns under new headers like xFe2O3 and xFeO.

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)

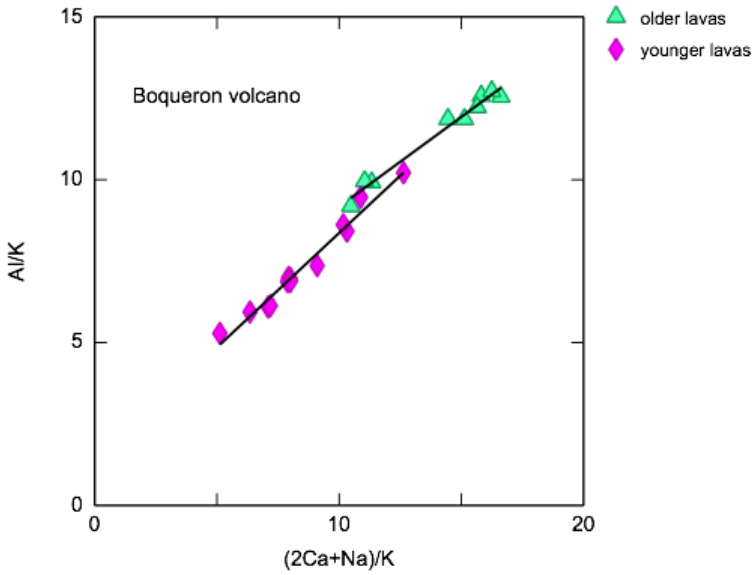
Commonly used calculations can be stored here and automatically made, rather than using Igpet's calculator. The data file "EXTRA.txt" is described in Appendix A. It includes a few standard parameters. The parameter FeO* is FeO+0.8998* Fe_2O_3 and it has not been normalized. Mg# is 100*MgO/(MgO+FeO+0.8998* Fe_2O_3), where the oxides are first divided by their molecular weights. Ba/La and La/Yb are just what they say. Ce*, Eu*, Nb* are normalized values obtained by log interpolation from adjacent REEs. The epsilon Nd value at zero age is eNd_o. The value of CHUR is set to 0.512638 and the o subscript indicates that this is a zero age calculation.

There are two built in parameters. Density is calculated on a normalized basis with 88% of total Fe as FeO, 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.txt". Fairbrothers et al. (1978) showed that an older suite at Boqueron had a calcalkaline fractionation path caused by removal of nearly equal proportions of plag and cpx {pl/(cpx+pl)=0.55}; whereas the recent lavas had a tholeiitic path 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). The slope of the regression should be pl/(pl+cpx) and ol will have no effect. 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, the slope for the older lavas is 0.551. For the younger suite the slope is

0.703. Although statisticians caution against PER diagrams (see Rollinson, 1993 for summary), sometimes this method produces results compatible with other approaches.

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 text files (.txt) or comma delimited text files (.csv). Both are ASCII or flat text files. 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.

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.				

Comma delimited data file structure

Replace all the tabs with commas and the .csv files are almost like the .txt files. The difference is that some column headers (variable names) or alphabetic data can have commas in them. Excel knows to bracket such items in quotes, e.g. "Basalt, tholeiitic." This makes dealing with .csv files more difficult, because software has to recognize the quotes and take steps to handle what follows. Regardless of file type, 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 **7 reserved words**, two of which, Sample (actually the string "samp") and Kcode, should be included in any file.

Sample	the sample name, a string variable
Mineral*	mineral abbreviation, ol, opx, cpx, pl, hb, mt, il, rut, ga, phl, etc
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 drawing error bars, the error in the previous column e.g. SiO[2] error 51.3 .513 for a 1% error in SiO_2
*	**for Mineral files only, not for rocks**

Using Igpet's File Operations

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

View data A grid is presented with all the data up to 64 column limit.

Save file **Warning! Use a new name!**
The file save dialog box opens and you select a new name and extension, if needed.

Add a file (Merge Files) **THIS IS OFTEN VERY VERY USEFUL**
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 (columns) that the first file lacks, these data fields will not be part of the new joint file unless you first add dummy to the first file using the same column headers as are in the second file. This option is useful for merging files with data in different order.

Data files to and from spreadsheets via .txt files
Excel and other spreadsheets can write **tab or comma delimited txt files**. Use Excel to maintain your data in the default format (*.xls or *.xlsx). When you are ready to make plots, save the data file as a tab or comma delimited text file (a *.txt or csv file). Use your spreadsheet to update data files; it is much more efficient than a text editor. Comma delimited files (.csv) appear to be the native format for data extracted from GEOROC. Therefore, Igpet now reads these files. However, GEOROC often has empty columns that greatly expand the number of variables in Igpet. These show up as empty buttons on the variable menu. I suggest saving the raw GEOROC extract to a tab delimited file and then removing all the empty columns and blank rows, if present. You should also add a Kcode column to assign a variety of symbols to each subset of the data.

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*, ∑Nd). Earlier versions of Igpet allowed one to formulate these derived parameters but the logic was awkward. The Text box calculator, 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 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.

Mineral Diagrams (in MIN Folder)

A few simple mineral plots are created by the control file Minplot.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. Third is a string of mineral abbreviations, connected by "+". Finally, there is a placeholder for the 4th place. The mineral abbreviations identify the minerals that will be plotted. Igpet compares the strings separated by the "+" signs to the Mineral column in the data file. 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      dummy
En    MgO
Wo50  CaO
Fs    FeO+MnO
0     1     0     .5     0     1
0
0
```

There are also mineral strings in the partition coefficient (PC) files. So, it is a good idea to coordinate your mineral names in the PC file with the mineral strings in the Mineral column of your data files.

The default strings are: ol, opx, cpx, pl, hb, sp, mt, il, rut, ga, phl. You can change these to suit your preferences, just do so systematically in the mineral data files and the mineral diagram files, so that all appropriate minerals get identified and plotted and, also, the PC files, so that the Mixing app will be able to match partition coefficients and minerals.

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 plagioclase projections from the Grove groups's publications include the results of Sack et al. (1987). This results in a straighter cpx-ol boundary, near the cpx-ol sideline. The Grove projections generally assume all Fe is FeO. To allow for this the Igpet versions of the logic add 0.899 times Fe_2O_3 to FeO. This is useful for rock analyses by XRF where all Fe is treated as Fe_2O_3. Grove projections also use quantities like $AlO_{1.5}$. For ease of programming these expressions are kept in mole units and multiplied by 2, so 0.5* $AlO_{1.5}$ = Al_2O_3.

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.

Discrimination and classification diagrams (in Diagrams folder)
DiscrimBasalt.txt, Granite.txt, Komatii.txt, Mantle.txt, Rocktype.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. IrvineBaragar.txt is the Irvine and Baragar (1971) rock classification scheme. The diagrams and plotting parameters for the DiscrimBasalt file are mostly from Rollinson (1993). For proper use, these discrimination diagrams should be used only in conjunction with the original references or Rollinson (1993)! The index numbers refer to figures in Rollinson's Chapter 5. Pay attention to the limits set for all the diagrams. First of all DiscrimBasalts is for basalts, so use **SubSelect** to set maximum and minimum values for SiO_2. With rigor I use the TAS limits, 45 to 52. I sometimes relax that to include picro-basalts and basaltic andesites with TAS limits expanded to 41 to 57.

The IUGS commission on rock nomenclature sets the rules on how igneous rocks should be named (Le Maitre et al., 2002 and 2010). The IUGS specifies two diagrams based on modal analysis, QPAF plutonic and QPAF volcanic, for the majority of igneous rocks. A few special diagrams are defined for unusual igneous rocks. The primary diagrams are based on the percentages of minerals in the rock as determined by thin section analysis, either by point counting or by image analysis. This approach is more suitable for intrusive rocks, which commonly are completely crystalline. For volcanic rocks, the alternate method is to obtain

the chemical analysis and use a TAS diagram, total alkalies (Na_2O+K_2O) versus silica (SiO_2). Igpet is primarily aimed at chemical petrology so the most useful IUGS diagram is the TAS diagram in the file, IUGS2002Chemical, in the Diagrams folder. IUGS2002Modal requires modal analyses. The mineral names Igpet looks for are: plagioclase, orthopyroxene, clinopyroxene, olivine, hornblende, quartz, feldspathoids (a combination- see ref) and alkali-feldspar (another combination). The online version of Le Maitre et al., (2010) should be read carefully. Igpet does not fully implement the IUGS recommendations, which are quite complex.

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 $^{87}Sr/^{86}Sr$ ratio to calculate ppm ^{87}Sr and ppm ^{86}Sr. The values for each endpoint go into the equation for determining the coefficients of the hyperbola. For Nd, Pb and Hf 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 X-Y Model option, is identical to the line from the Mix button for two endpoints, but can't extend beyond the endpoints. 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.TXT, 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 3 6. 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 View. 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 TextEdit to fix the problem.

Points are shifted right in the TAS diagram
This diagram was designed by the authors using data normalized to 100% water free with all Fe as FeO. Most analyses sum to less than 100% without water so normalization often shifts SiO_2 to noticeably higher values. This is not a problem.

Too Many Fe parameters
Some data sets include Fe_2O_3 and FeO where both are determined separately. This is the correct presentation but it is no longer common. Most modern data sets have only Fe_2O_3 or only FeO with the other oxide set to zero. This is the best situation for Igpet, which has built in routines for apportioning the Fe between the two oxides. Serious error occurs if the data set includes both oxides and puts all the Fe into both. Some Igpet functions use both Fe oxides so putting all the Fe into both Fe-oxide columns doubles the amount of Fe seen by the Igpet functions and causes error.

Failure of International awareness
Igpet tries to read data files in the format appropriate for each country. In the United States the period is the decimal marker but in many other countries it is the comma. A function called CStr id supposed to take care of this but it sometimes fails. Therefore Igpet has a backup routine that recognizes the period as the decimal marker, so a file in US format can be read by Igpet regardless of the International setting. If you data file fails to read properly, save a new version after changing the format to US settings (period as decimal marker and no other punctuation for numbers.

Mixing.app

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. Therefore, some successful appearing fits may be nonsense. The best you can say of a model with low residuals is that it has not been rejected, but it certainly cannot 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). If you will be ignoring trace elements select Null.PC.txt. Next, select a weighting function for oxides file (.wt.txt). Click the View PCs button and note that there is 0 weight for Fe_2O_3. This is a reminder that Mixing puts all the Fe in to FeO. Now read a mineral file and a rock file. You can read new mineral, rock or PC.txt files at any time.

The partition coefficient files hold the partition coefficients needed for trace element calculations. The weights files hold the weighting values for the major oxides. 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). Trace elements do not contribute to the solution but can help as a separate check on the solution. Incompatible elements behave well because they are simply concentrated in the residual liquid. In the Raleigh equation F is % liquid, the Cs are concentrations and D is the weighted sum of partition coefficients, the bulk partition coefficient of the cumulate crystals. The Raleigh equation is $C_{liq} = C_o \cdot F^{(D-1)}$. For incompatible elements (e.g. those with D values near zero) the equation simplifies to $C_{liq} = C_o/F$. For compatible elements, those strongly partitioned into phenocrysts (D>1), the changes in concentration as F decreases are very large and very susceptible to error in partition coefficients.

View PCs, button at the lower left, lists 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 the mineral file you read. One of these strings needs to match the mineral abbreviations in the Mineral column of the data file 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" in the column labeled “Mineral.”

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.

Now load data files and begin making models. Start with Gill.PC, CerroNegroGeochem and cerronegro.min and reproduce the 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).

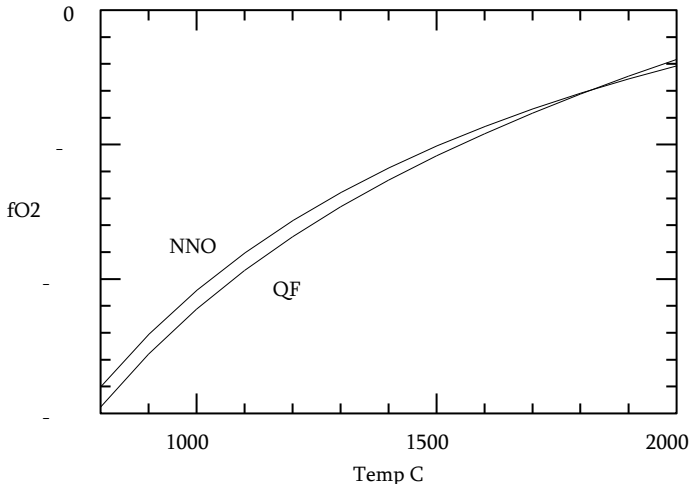
The result is seen as soon as you finish your selection. Output goes first to the screen, but you can send a copy to a text file or a corrected rock file. The last option allows you to build a file of fractionation corrected data, which is useful for trace element modeling.

PTfO2.app

This interactive program demonstrates how Fe_2O_3 and FeO vary depending on composition (X_i) and assumptions made about pressure and the appropriate oxygen buffering. Temperature is calculated from X_i and P following the equations of Beattie (1993). Oxygen buffers (NNO, QFM and IW) and pressure (P in Gpa) can be selected and the T, P, and fO_2 are then used to partition Fe between Fe_2O_3 and FeO following Kress and Carmichael (1991). Because the T logic is based on partitioning of Mg/Fe between olivine and melt, this logic is primarily for basalts and more mafic magmas in the temperature range 1000°C to 2000°C. Results for silicic rocks are likely to be highly unreliable.

The fO_2 buffers used are:

NNO (O'Neill and Pownceby, 1993)
fo2 = (-478967 + 248.514 * T - 9.7961 * T * Log(T)) / (8.31441 * T * 2.302585)
QFM (O'Neill, 1987)
fo2 = (-587474 + 1584.427 * T - 203.3164 * T * Log(T) + 0.09271 * T ^ 2) / (8.31441 * T * 2.302585)
IW (O'Neill and Pownceby, 1993)
fo2 = (-550915 + 269.106 * T - 16.9484 * T * Log(T)) / (8.31441 * T * 2.302585)



Appendix A: Control Files

Igprefini.txt and **Igpetdata.txt**
These files control the IGPET system. You should modify **Igprefini.txt** 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+++ (no longer used)
{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 in the normalization used in the S-Norm button on the 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

Default.sym.txt is the file Igpet loads initially to make symbols. Symbol files are tab delimited with 6 columns, the last of which is a polygon, a circle or a line definition. There are two colors, line and fill, that can easily be customized. Using Excel one can move things around and insert new colors. Shapes or polygons can be designed using graph paper. The polygon units are 1/1000 of an inch. The first number is a global scale factor takes the raw polygons and expands (not a good idea) or contracts them all. There is room for 36 symbols!

Lines and symbols are created from six columns of alphanumeric data. The first two, number and description, are not used but are needed as place holders. Line color|width is a color R|G|B|, followed by a width of 15. Fill color is an RGB group, R|G|B. Shape type is self-explanatory. The 6th column is a definition of a circle, polynomial or line.

number	description	Line color|width	Fill color	ShapeType
0.5	scale factor for symbols	x	x	x
14	font size	x	x	x
1	tickpencolor-width	0|0|0|15	x	x
2	mixmodpencolor-width	0|0|0|20	x	x
3	pagecolor	255|255|255	x	x
4	boxcolor	255|255|220	x	x
5	textcolor	0|0|0	x	x
-1	openCircle for ticks	0|0|0|1	0|0|0	CIRC
0	openCircle	0|0|0|1	0|0|0	CIRC
1	openTriangle	0|170|85|15	255|255|255	POLY
……	filledCircle	225|0|0|1	255|0|0	FCIRC
9	+	0|0|0|15	0|0|0	LINE
10	asterisk	0|0|0|15	0|0|0	LINE

Circle, polygon and line examples

CIRC 1|50|50 defines a circle with one xy pair which defines a radius of 50
POLY 4|130|-74|0|152|-130|-74|130|-74 defines a polygon with 4 points (a triangle)
FPOLY 5|-112|-112|112|-112|112|112|-112|112|-112|-112 filled polygon with 5 points (a box)
LINE 6|0|-112|0|112|0|0|112|0|-112|0|0|0 line form made of 6 points (a plus sign)

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.

PercentFs.txt

This file sets the suggested F values (in percent) for common melt and crystallization models.

Fs_AFC_r=1	0,10,20,30,40
Fs_AFC_r<1	100,95,90,85,80
Fs_AFC_r>1	100,110,120,130
Fs_Equimelt	1,5,10,15,20,25
Fs_FracMelt	.1,.5,1,5
Fs_AggFracMelt	1,5,10,15,20,25
Fs_ContinMelt	.1,.5,1,5
Fs_RayFracXtal	100,90,80,70,60
Fs_EquiXtal	100,90,80,70,60
Fs_InSituXtal	90,70,50

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 two fixed items, density and viscosity. Density is calculated on a normalized basis with 88% of total Fe as FeO, using the method of Bottinga and Weill (1970) on a water-free, 1 atm, 1200° C basis. Viscosity estimates are at with 2% water and 1000° C after Giordano et al. (2008).

The eNd_o parameter assumes zero age! Do not use this for older rocks! Create your own ep_Nd values using Exel. Save calculated epsilon values as ep_Xy, where Xy is an element with isotope ratios like Sr or Nd.

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[o]	nozeros	"{143}Nd/{144}Nd"*10000/.512638-10000
Nb/Nb+	nozeros	(Nb/0.713)/((U/0.021)*(K2O*8301/250))^0.5
Nb/Nb*	nozeros	(Nb/0.713)/((Th/0.085)*(La/0.687))^0.5
Eu/Eu*	nozeros	(Eu/0.058)/((Sm/0.153)*(Gd/0.2055))^0.5
Ce/Ce*	nozeros	(Ce/0.612)/((La/0.237)*(Pr/0.095))^0.5

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* is an interpolation between Th and La.

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 files, 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
……..several lines cut
```

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 2nd to last entries in the first line define which minerals to plot. There is some flexibility.

```
MTRI    Feldspars       PL+FS+OR+ab+an          Feldspars
Ab      2*Na2O
Or      2*K2O
An      CaO
0       1       0       1       0       1
24
0       0.1     0
0.5     0.1     1
0.577708491     0.132783019     1
0.597891038     0.212617925     1
etc
MTRI    Pyroxene Quadrilateral  CPX+opx         Pyroxenes
En      MgO
Wo50    CaO
Fs      FeO+MnO
0       1       0       0.5     0       1
12
0.95    0.05    0
0       0.05    1
0.475   0.05    0
etc
```

CMAS folder

The format of these files is slightly different from that for the triangular files for regular diagrams. The diagram's 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 Cr2O3 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.

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 plots. 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.TXT 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. The partitioning of Fe between Fe++ and Fe+++ was calculated using the equation from Kress and Carmichael (1991) and the T and fO_2 data in the original publications.

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

key	symbol	ref.	description
4	filled box	Walker et. al., 1979	OFZ
7, 8	circles	Grove et al., 1982	Med._Lake, opx, cpx
11	asterisk	Grove and Bryan, 1983	Famous
2	filled triangle	Baker and Eggler, 1983	Atka
30	red stars	Sack et al., 1987	alkaline etc

COTHI.TXT contains 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. Fe was not partitioned in the high pressure results because the use of a graphite layer in the experimental charge prevented the formation of detectable Fe_2O_3.

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. An even larger file is available on the Smithsonian web site.

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

CAVF.TXT

see: Carr et al. (1990)

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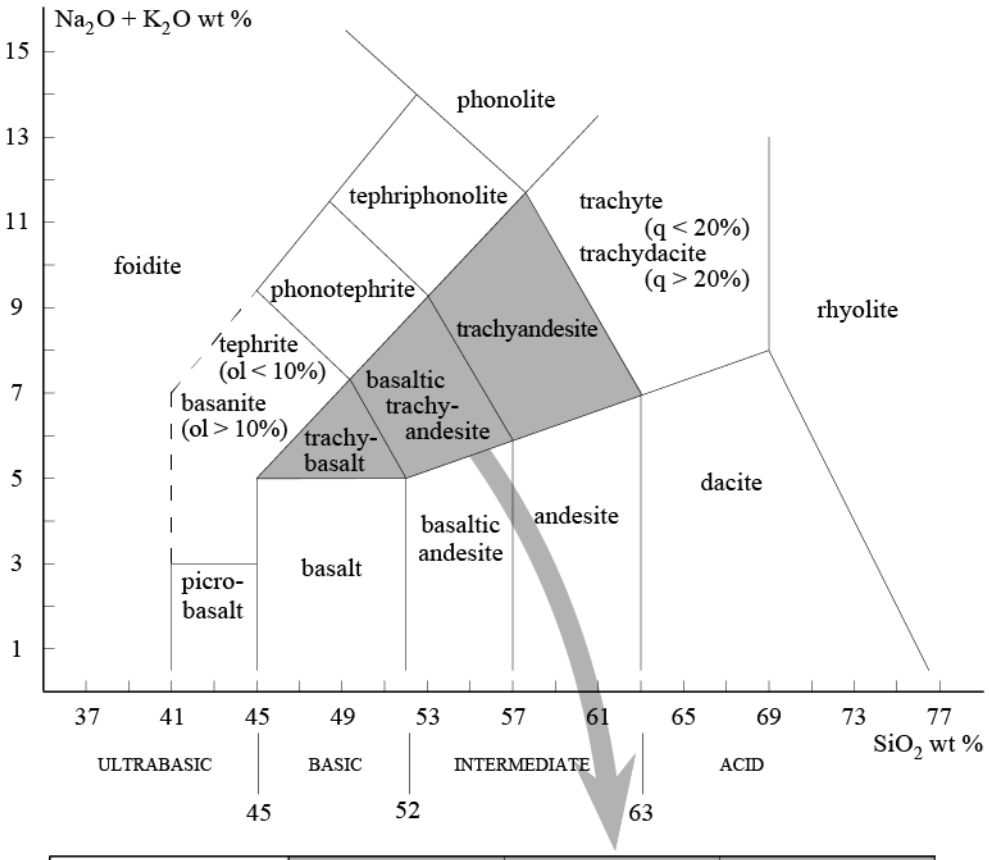
Appendix D: IUGS diagrams

Following diagrams from Le Maitre et al. (2002)



Further subdivisions of shaded fields	trachybasalt	basaltic trachyandesite	trachyandesite
$Na_2O - 2.0 \geq K_2O$	hawaiite	mugearite	benmoreite
$Na_2O - 2.0 < K_2O$	potassic trachybasalt	shoshonite	latite

Fig. 2.14. Chemical classification of volcanic rocks using TAS (total alkali–silica diagram) (after Le Bas et al., 1986, Fig. 2). Rocks falling in the shaded areas may be further subdivided as shown in the table pointed to by the arrow. The line between the foidite field and the basanite–tephrite field is dashed to indicate that further criteria must be used to separate these types. Abbreviations: ol = normative olivine; q = normative 100 * Q / (Q + or + ab + an).

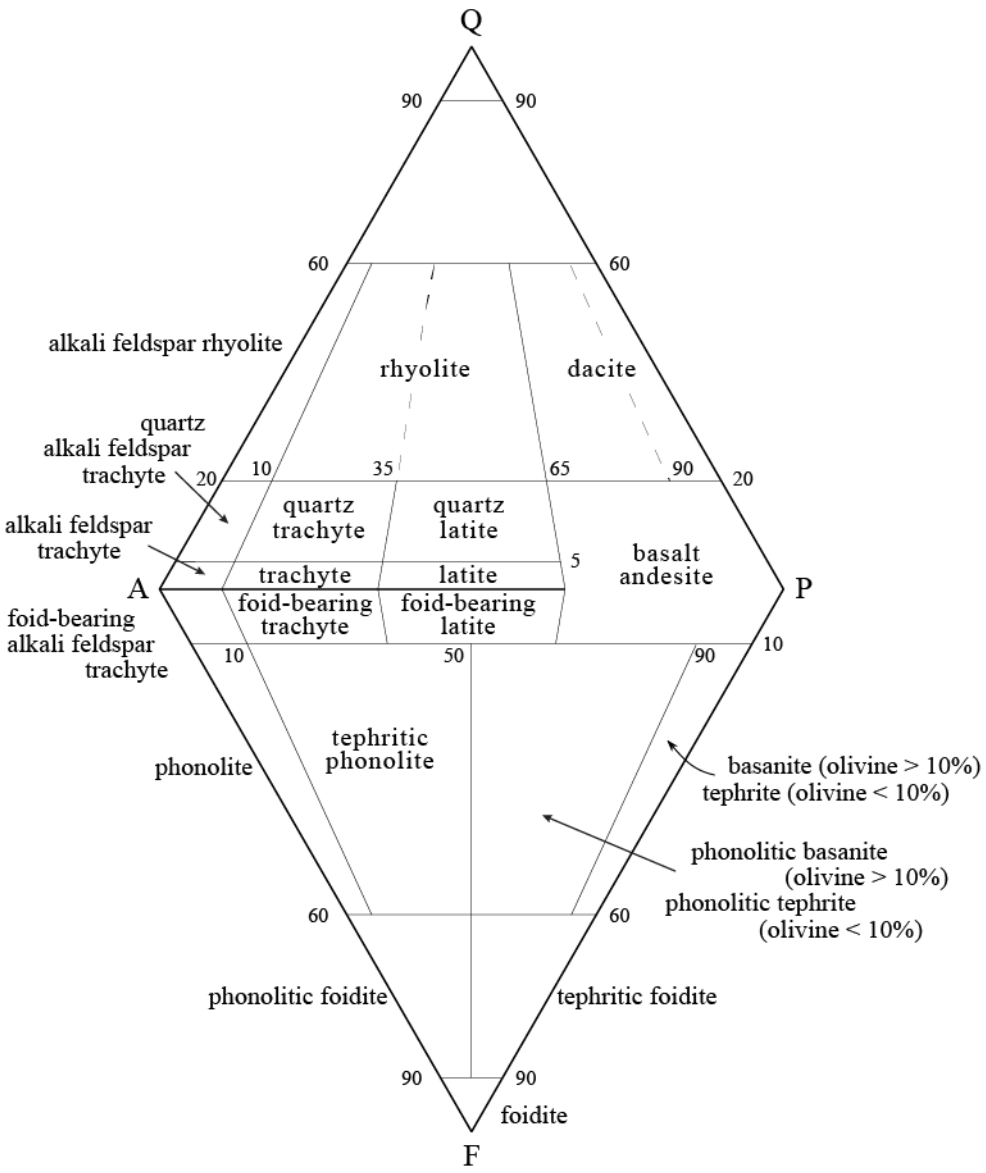


Fig. 2.11. QAPF modal classification of volcanic rocks (based on Streckeisen, 1978, Fig. 1). The corners of the double triangle are Q = quartz, A = alkali feldspar, P = plagioclase and F = feldspathoid. This diagram must not be used for rocks in which the mafic mineral content, M, is greater than 90%.

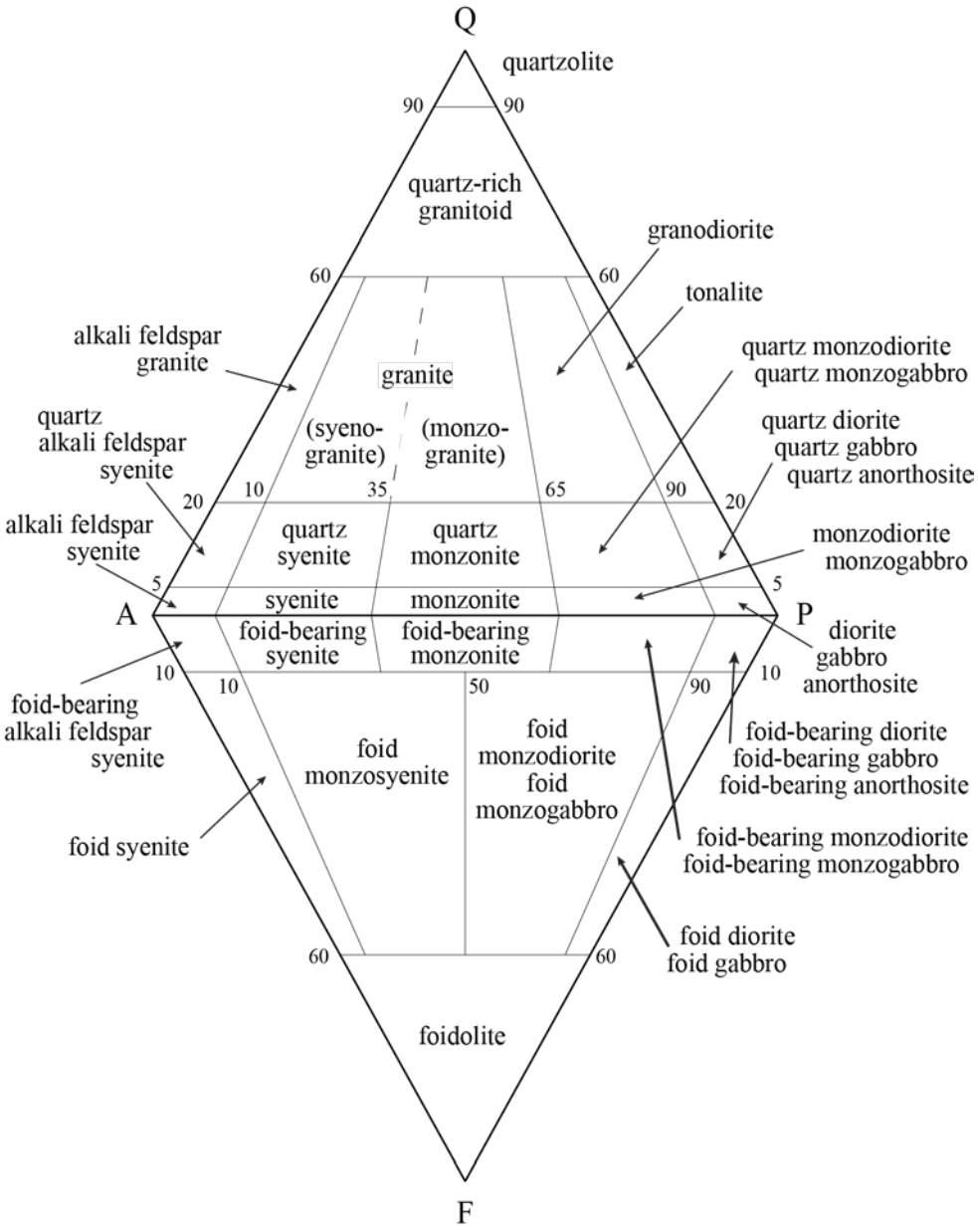


Fig. 2.4. QAPF modal classification of plutonic rocks (based on Streckeisen, 1976, Fig. 1a). The corners of the double triangle are Q = quartz, A = alkali feldspar, P = plagioclase and F = feldspathoid. This diagram must not be used for rocks in which the mafic mineral content, M, is greater than 90%.