

TABLE OF CONTENTS

Table of Contents	2
Main Features	3
1 Introduction	3
2 Open, Import, and Save files	4
2.1 Open .peg Files	4
2.2 Import Excel Files	4
2.3 Import Igpetwin Files	6
2.4 Save File	6
3 Plots & Diagrams	6
3.1 Generals	6
3.2 Binary Plot	6
3.3 Triangular Plot	7
3.4 Spiders	8
3.4.1 REE Spiders	8
3.4.2 Other Spiders	9
3.5 Classification and Discriminating Diagrams	11
3.6 Double click on graph	12
3.7 Right click on graph	12
3.8 Export plots & diagrams	13
4 Geochemical Models	13
4.1 Generals	13
4.2 Major Elements Models	13
4.2 Trace Elements Models	15
4.3 Isotope Models	17
5 Additional Features	18
5.1 Partition Coefficient Database	18
5.2 Operations and Filters	18
Examples	21
1 Import file and make a plot	21
2 Make a REE spider	25
3 Make a Model for Major Elements	26
4 Make a Trace Elements model	32
References	34
Credits	37

MAIN FEATURES

1 Introduction

Petrograph (see Figure 1 for a screen shot) is a program specifically developed to help the user to visualize, elaborate and in particular to model geochemical data. The source code is written in MS Visual Basic $6.0^{\text{®}}$ and it runs under Windows 98/2000/XP[®] platforms.

The software is able to plot data on several different diagrams, including a large number of classification and 'petro-tectonic' plots. Petrograph gives the opportunity to manage large geochemical datasets in a single program without the need of passing from one software to the other as usually happens in petrologic data handling. Along with these basic functions, Petrograph comes with wide choice of modelling capabilities from major element mass balance calculations to the most common trace element and isotope models. Results and graphs can be exported as vector graphics in publication quality form or they can be copied and pasted within the most common graphics programs for further modifications. All these features makes of Petrograph one of the most complete software presently available for igneous petrology research.

Petrograph can be downloaded from the following URL:

http://www.unipg.it/~maurip/SOFTWARE.htm



Figure 1

2 Open, Import, and Save files

2.1 Open .peg Files

The option "open" allows to open ".peg" files previously saved using Petrograph. To open a .peg file, select the option "Open" from the "file" menu or click the button 🖾 in the control bar.

2.2 Import Excel Files

To open a .xls file, select the option "import – file Excel (.xls) from the "file" menu or click the button in the control bar. Before importing an Excel worksheet, ensure that data are correctly arranged. Data can be easily arranged in the Excel worksheet following these rules (Figure 2): - the first column must contain the sample name;

- a number between 0 and 12 must be placed in the second and the third column. These numbers correspond to the symbol and the colour used to plot the sample, respectively;
- the fourth column must contain the number zero (0) or one (1); if Petrograph encounters 0, it will not display the sample in diagrams;
- the first row must contain the name of analysed elements, isotope, etc...
- if some data are not available, the symbol "-" must be used;
- the syntax for the isotope ratio must be as follow: "wheight of the isotope"+"Element"+"/"+ "wheight of the isotope"+"Element" (for example the ratio between the isotope 87 and 86 of Strontium (Sr) must be written as 87Sr/86Sr.



- the first column must contain the name of the sample; - a number between 0 and 12 must be placed in the second and the third columns. These numbers correspond respectively to the symbol and the colour used to plot the sample.

2

1

c

64 1

6

Sample 5

In E

-The fourth column must contain the numbers zero (0) or one (1); if Petrograph finds 0 it will not display that sample, on contrary if Petrograph find 1 it will display it All these parameters can be changed within Petrograph

common analytical output in the case that analyses are below the detection limit)

2.3 Import Igpetwin Files

Igpetwin is a widely diffused program to plot and manage geochemical data. This program saves data files using the .roc extension; Petrograph is able to recognize the structure of .roc files and imports these files without any further arrangement. To import a .roc file, select the option "import – file IgpetWin (.roc) from the "file" menu or click the button in the control bar.

2.4 Save File

This option allows to save the data. Petrograph saves files using the .peg extension. To save a file, select the option "save" from the "file" menu or click the 🖳 button in the control bar.

3 Plots & Diagrams

3.1 Generals

Petrograph performs three type of diagrams: Binary, Triangular and Spider diagrams; it can also perform a large number of classification and discriminating diagrams.

3.2 Binary Plot

Plot a graph in y vs. x coordinates.

To perform a binary plot, open the "binary plot windows" (Figure 3) selecting the option "binary plot" from the "Plot" menu or clicking the button in the control bar.

Elements for the x and the y axes can be selected using the buttons and the diagram can be created by clicking on the button "Plot (Spacebar)".





3.3 Triangular Plot

Plot a triangular plot.

To perform a triangular plot, open the "triangular plot window" (Figure 4) selecting the option

"triangular plot" from the Plot Menu or clicking the button *i* in the control bar.

Elements for the A, B and the C corners can be selected using the buttons and the plot can be created with a click in the button "Plot (Spacebar)".



Figure 4

3.4 Spiders

3.4.1 REE Spiders

Plot a spider of Rare Earth Elements (REE, Figure 5).





To perform a REE spider plot, open the "REE spider window" (Figure 6) by selecting the option "Spider - REE" from the "Plot" menu or clicking the button in the control bar. It is possible to plot a maximum number of 50 samples contemporaneously by selecting them using the button in. Several option are available to customize a spider diagram. Among these, the possibility to change values the normalizations (see Table 1) by selecting the preferred values in the relative cascade box; selected normalization values will appear on the right side of the window. To create the diagram, click the button "Plot (spacebar)".

Samples Selection	REE spiders		×	Í.
2	Spider List (max 6	50) Normalizi	ing Value	
	- add - 3	La	.33	7
Green box:	Etements Media Ene M 310Ene D	- Ce	.88	
Red Box:	La Sm Ho Media Enc D	Pr	.112	
REE not available	Ce Eu Er 63HbBTon	Nd	.6	
	Pr Gd Tm 127HbBTon	Pm	1	
	Nd Th Yb	Sm	.181	
Normalization	Pm Dy Lu Remove sample	Eu	.069	
selection	Congris or NASC	Gd	.249	_ Normalization
selection	Ontions	ть	.047	values
	Graph Dim. (pixel) Symbol Width	Dv	1	
	Width 500 1 I Line Widt	h Ho	07	
	Symbol Dim	- Fr	2	
	Height 300 Med -	Tm	03	
Create the		Yb	2	
spider diagram 🏊	Plot (SpaceBar) Cancel	Lu	.034	



3.4.2 Other Spiders

Plot a spider diagram.

To perform this type of diagram, open the "Other spider window" by selecting the option "Spider -Other" from the "Plot" menu or clicking the button in the control bar. Figure 7 explains the features of the "Other spider window".



Figure 7

Several normalization for the Primordial Mantle, Condrite, MORB and crust can be selected (see Table 1) and it is also possible to import a personal normalization file. Personal normalization are text files formatted as described in (Figure 8).

REE Spiders
- Chondrite - Haskin et al.(1968)
- Chondrite - Masuda et al.(1973)
- Chondrite - Nakamura (1974)
- Chondrite - Boynton (1984)
- Chondrite - Sun & McDonough (1989)
- NASC - Haskin & Frey(1966)
- NASC - Haskin & Haskin(1966)
Other Spiders
- Primordial mantle - Wood et al. (1979a)
- Primordial mantle - McDonough et al. (1992)
- Primordial mantle - Taylor & McLennan (1985)
- Condrite - Wood et al. (1979b)
- MORB - Bevins et al. (1984)
- Upper cont. Crust - Taylor & McLennan (1981)
- Lower cont.crust - Weaver & Tarney (1984)
- Average cont crust - Weaver & Tarney (1984)
 Average N-type MORB - Saunders & Tarney (1984); Sun (1980)
- Average OIB - Sun (1980)
Custom Spider (allows to generate personal normalization file)

Table 1



Figure 8

3.5 Classification and Discriminant Diagrams

Petrograph performs a large number of classification and discriminating diagrams (see Table 2). To plot one of these diagrams, select the option "diagram" from the "plot" menu or click the button **in the control bar.** A list of diagrams, divided by categories, will appear. Now select the diagram of interest to plot it.

General Classification Diagrams

Binary [Q'(F')-ANOR] - volcanic - after Streckeisen & LeMaitre, 1979 [K₂O-SiO₂] - after Peccerillo and Taylor, 1976 [K₂O-SiO₂] - after Peccerillo and Taylor, 1976 [K₂O-SiO₂] - after Middlemost, 1975 [TAS Alkalies-Silica] - volcanic - after LeBas et al., 1986 [TAS Alkalies-Silica] - volcanic - after Cox et al., 1979 [TAS Alkalies-Silica] - plutonic - after Cox et al., 1979 [SiO₂-K₂O Andesite Types] - after Gill, 1981 [SiO₂-F/M] - after Miyashiro, 1974

> *Triangular* AFM - after Kuno,1968 AFM - after Irvine & Baragar, 1971

Diagrams for Basalts

Binary [Ti-Zr] - after Pearce & Cann, 1973

Triangular [Ti-Zr-Y] - after Pearce & Cann, 1973 [Ti-Zr-Sr] - afterPearce & Cann, 1973 [Nb-Zr-Y] - after Meschede, 1986 [Th-Hf-Ta] - after Wood, 1980

Diagrams for Granites

Binary [Nb-Y] - after Pearce et al., 1984 [Ta-Yb] - after Pearce et al., 1984 [Rb-(Y+Nb)] - after Pearce et al., 1984 [Rb-(Yb+Ta)] - after Pearce et al., 1984

Table 2

3.6 Double click on graph

By double Click on a diagram the user can change some attributes of a graph. The nature of possible changes is function of the selected graph. For example a double click on the binary plot open the windows displayed in Figure 9. This window allows to adjust the maximum, the minimum and the step interval for the axes; it also permits to change plotted elements and it allows to change the dimension of the window in which the graph is displayed.

AXIS X			AXIS Y		Graph Dim. (picel)		
MgO		•	CaO		·	Width 500	
Max. X:	5		Max,Y:	9			
Min. X:	0	_	Min. Y:	0	_	Height] 300	
Step X:	0.5		Step Y:	1	-	Constitution	
Log/Norm:	LIN	· · ·	Log/Norm:	LIN		Operation	

Figure 9

3.7 Right click on graph

By right click on a graph a cascade menu containing some possible actions appears (Figure 10). For example, it is possible to copy the diagram in the clipboard, to insert a trace element model, to change the shape of the symbols and their colours etc...



Figure 10

3.8 Export plots & diagrams

To export a graph, the user can copy it in the clipboard and successively paste it in another application or he/she can save it as Windows Metafile image (.wmf). To copy the diagram, click the right button on the selected plot and click on "Copy Graph" from the cascade menu (Figure 10). To save the diagram, proceed as for the "Copy Graph" option but select "Save Graph (.wfm)" from the cascade menu (Figure 10).

4 Geochemical Models

4.1 Generals

One of the principal features of Petrograph is the possibility to perform geochemical models for major, trace elements and isotopes.

4.2 Major Elements Models

Major elements are modelled by using the mass balance algorithm by Stormer and Nichols (1978). To start a mass balance calculation, open the "Mass Balance Window" by selecting the option "Mass Balance" from the "Windows" menu or clicking the button Σ in the control bar. Figure 11 explains the main features of the "Mass Balance Window".

	Sele	Select Oxides		elect Magma	hases]		
	Initial Magma	Final Magma	HB19	9 AB	All			
5102	40.35	67.04	35.4	68,74	43.19			
102	1.39	0.43	3.8	0	0			
1203	15	15.6	12.1	19.44	36.65			
eOtot	12.24	2.54	18.5	0	0			
4n0	0.19	0.04	0.2	0	0			
0ph	8.94	1.29	14.8	0	0			
aO	8.93	3.96	12.2	0	20.16			
la20	3.2	4.61	1.4	11.82	0			
20	0.92	2.36	0	0	0			
TOT	39.46	97.07	98.4	100	400			
OUTPU	T DATA	Tar ar		j	hoo			
OUTPU SUM OF	T DATA	THE SQUAP	ES OF	F THE	RESIDUALS		1.511	
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UTPU SUM OF PHASE NAME HB199	T DATA	THE SQUAP MOUNT AS VT.% OF NIT. MAGM -58:	ES OF 3 AN W A AL 198	F THE MOUNT AS T.% OF LL PHASES 82.923	RESIDUALS AMOUNT AS WT.% OF ADDED PHS.	AMOUN WT.% C SUBTR	1.511 NT AS DF D.PHS. 82.923	
UTPU SUM OF PHASE NAME HB199 AB	T DATA	THE SQUAF MOUNT AS VT.% OF NIT. MAGM -58: -8	ES OF 3 AN W A AL 198 406	F THE MOUNT AS T.% OF LL PHASES 82.923 11.978	RESIDUALS AMOUNT AS WT.% OF ADDED PHS. 0	AMOUN WT.% C SUBTR	1.511 NT AS DF D.PHS. 82.923 11.978	
UTPU SUM OF PHASE NAME HB199 AB AN	T DATA	THE SQUAP MOUNT AS VT.% OF NIT. MAGM -58. -8. -3.	ES OF 3 AM W A AL 198 406 579	F THE MOUNT AS T.% OF LL PHASES 82.923 11.978 5.1	RESIDUALS AMOUNT AS WT.% OF ADDED PHS. 0 0 0	AMOUN WT.% C SUBTR	1.511 NT AS DF D.PHS. 82.923 11.978 5.1	
UTPU SUM OF PHASE NAME HB199 AB AN		THE SQUAP MOUNT AS VT.% OF NIT. MAGM -58. -8. -3. () INITIAL	ES OF A AL 198 406 579 M4	F THE MOUNT AS T.% OF LL PHASES 82.923 11.978 5.1	RESIDUALS AMOUNT AS WT.% OF ADDED PHS. 0 0 0	AMOUN WT.% C SUBTR	1.511 NT AS DF D.PHS. 82.923 11.978 5.1 70.183	

Figure 11

The mass balance algorithm involves a least-squares solution to a set of linear mass-balance equations (one for each oxide) and the calculations are performed on data consisting of chemical analyses of igneous rock, assumed to represent the composition of "magmas", and chemical composition of minerals or other rocks, assumed to represent "phases" added or subtracted from one "magma" to derive a second "magma". As described by Stormer and Nicholls (1978), this computation can be used to test fractional crystallization (by subtraction of analysed phenocrysts or cumulate minerals as "phases"), assimilation (by addition of country rock as "phase"), fractional melting (by subtraction of residual minerals or refractory residual rock "phases" from an assumed parental rock "magma"), and magma mixing (by adding a third magma, entered as a "phase" to the

first "magma" to derive a second "magma"). Mass balance computations are performed in a user friendly environment (Figure 11) by selecting "magmas" and "phases" among the samples belonging to the geochemical dataset and the output is reported in the same way of the original program of Stormer and Nichols (1978; see the Examples section for more details about the mass balance computation).

4.2 Trace Elements Models

Trace element models are very useful to quantitatively discriminate among different geochemical processes mostly because they are dilute and their behaviour depends primarily on the element-matrix interaction and very little on the element-element interaction. This implies that geochemical processes for trace element can be modelled using simple equations. Several trace elements models are implemented in Petrograph and they are divided in three main sections: (i) models related to the crystallization process (Table 3), (ii) models related to the melting process (Table 4a) and finally (iii) one model for the mixing process (Table 4b).

Trace elements models are performed by Petrograph directly on binary plots. To develop a trace element model, select "Insert Model" from the cascade window generated by a right click on the diagram (Figure 10). Melting and Crystallization models can be performed by selecting the option "Models Generator" whereas for the mixing process select "Mixing" (see the Examples section for more detail on the trace element models development).

Model (Reference)	Sigle	Equation	Parameters				
Equilibrium Crystallization (Wood & Fraser, 1976)	EC	$C_L = \frac{C_o}{[D + F(1 - D)]}$	C _L C _O D F	 concentration of trace element in the melt initial concentration of trace element bulk partition coefficient fraction of melt remaining 			
Fractional Crystallization (Neuman et al., 1957)	FC	$C_{t} = C_0 F^{(D-1)}$	C _L C _O D F	 concentration of trace element in the melt initial concentration of trace element bulk partition coefficient fraction of melt remaining 			
Assimilation plus Fractional Crystallization (DePaolo, 1981)	(AFC	$\begin{split} \widetilde{C}_{L} &= C_{D} \Bigg[f'' + \frac{r}{(r-1+D)} \cdot \frac{C_{A}}{C_{O}} \cdot (1-f'') \Bigg] \\ f'' &= F^{-(r-1+D)/(r-1)} \end{split}$	C _L C _O C _A F r	 concentration of trace element in the melt initial concentration of trace element concentration of trace element in the assimilated wallrock bulk partition coefficient fraction of melt remaining ratio of the assimilation rate to the fractional crystallization rate 			
In Situ Crystallization (Langmuir, 1989)	In Situ C	$C_t = C_o (M_t / M_o)^{\{f(D-1), \{D(1-f) \neq f\}\}}$	C _L C ₀ M ₀ D M _L	 concentration of trace element in the melt initial concentration of trace element initial mass of the magma chambers bulk partition coefficient mass of the liquid fraction of magma allocated to the solidification zone which is returned to the magma chambers 			
Zone Refining (Richter, 1986)	ZR	$C_{L} = C_{O} \left[\frac{1}{D} - \left(\frac{1}{D} - 1 \right) e^{-nD} \right]$	C _L C _O D	 concentration of trace element in the melt initial concentration of trace element bulk partition coefficient number of equivalent rock volumes that have reacted with the liquid 			

Table 3

a) Melting Models (Reference)	Sigle	Equation	Parameters
Batch Melting (Wood and Fraser, 1976)	ВМ	$C_L = \frac{C_O}{\left[D_{RS} + F(1 - D_{RS})\right]}$	C_L = concentration of trace element in the melt C_O = trace element concentration of the unmelted source D_{RS} = bulk partition coefficient of the residual solid F = fraction of melt produced
non Modal Batch Melting (Wood and Fraser, 1976)	nMBM P	$C_{L} = \frac{C_{O}}{[D_{O} + F(1 - P)]}$ $= p_{1}K_{1} + p_{2}K_{2} + \dots + p_{n}K_{n}$	C_L = concentration of trace element in the melt C_O = initial concentration of trace element D_O = bulk partition coefficient ρ = normative weight fraction of minerals in the melt κ = mineral / melt partition coefficient F = fraction of melt produced
Fractional Melting (Wood and Fraser, 1976)	FM	$C_{t} = \frac{C_{0}}{D_{0}} (1 - F)^{(1/D_{0} - 1)}$	C_L = concentration of trace element in the melt C_O = trace element concentration of the unmelted source D_O = bulk partition coefficient of the original solid F = fraction of melt produced
b) Mixing Model (Reference)	Sigle	Equation	Parameters
Mixing (Langmuir et al., 1977)	Mix	Ax + Bxy + Cy + D $A = a_{2}b_{1}y_{2} - a_{1}b_{2}y_{1}$ $B = a_{1}b_{2} - a_{2}b_{1}$ $C = a_{2}b_{1}x_{1} - a_{1}b_{2}x_{2}$ $D = a_{1}x_{2}y_{1} - a_{2}x_{1}y_{2}$	See Langmuir aet al., 1977 for detail

Table 4

4.3 Isotope Models

Regarding Isotopes, Petrograph can model the process of Mixing (Langmuir et al, 1978) and the process of Assimilation plus Fractional Crystallization (AFC; De Paolo, 1981). To develop a model for isotopes, select "Insert Model" from the cascade windows generated by a right click on the diagram (Figure 9). AFC model can be performed by selecting the option "Isotopic AFC" while for the mixing process select the "Mixing" option as for trace elements mixing.

5 Additional Features

5.1 Partition Coefficient Database

A partition coefficient database can be opened by selecting the option "Partition Coefficient DB" from the "Windows" menu. As result, the "Partition Coefficients Windows" will appear (Figure 12); the partition coefficients relative to an Element will be displayed by clicking on it. Data for the partition coefficient database are from Earth Reference Data and Models web site (EARTHREF; www.earthref.org).

н																н	He
u	Be											в	С	N	0	F	Ne
Na	Mg											AI	Si	P	s	CI	Ar
к	Ca	Sc	TÌ	۷	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Мо	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	T.	Xe
Cs	Ba		Hf	Та	w	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
Fr	Ra																
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Но	Er	Tm	Yb	Lu	
		Ac	Th	Pa	U												
														Hide	(Spac	:eBar)



5.2 Operations and Filters

The elaboration of variables stored in the original dataset can be performed by Petrograph using two principal types of operation: (i) mathematical operations and (ii) determination of geochemical parameters and indexes (Figure 13).

Mathematical operation are the sum, subtraction, multiplication, division, the elevation to an exponent, and the square root. These operations allow the user to generate new variables that can be plotted and/or further elaborated.

Geochemical parameters and indexes that can be determined by using Petrograph are: CIPW, Larsen Index, Solidification Index, Total Iron (FeOTot) and Fe/Mg Ratio; weight per cent value can be converted in molar value and Eu anomalies can be also calculated.

Select		202003	-	
Algebric	al Opera	tion	1	
A+B	A-B	AxB	A/B	
A*Cost	A/Cost	1/A	A*2	
SQR(A)	PPM>%	VVT 96V	VT>PPI	
Geocher	nical Ope	ration -		
FeOtot	Larsen	Index	S.I.	
CIPW	Mg	#	ASI	
Fe/Mg			mola	
REE Ope	eration	15		
Eu/Eu*	(La/S	m)N (1	La/Yb)N	
	(Tb/Y	b)N		
Condrite r	ormalizati	on:		
Haskin et	al.(1968)	2007	1	
Filters -				

Figure 13

To perform one of the above operations, select the "Operation" option from the "Windows" menu or click the button f in the control bar.

Regarding the CIPW Norm calculation note that Petrograph do not perform any adjustment for Fe molecular ratio (see Cox et al., 1979 and Best, 2003 for detail) and as benchmark for the computation the program computes the difference between the sum of the weight percentages of the oxides in the original analysis and the sum of the normative minerals. This value should be within (+/-0.2) the error due to the rounding operations. The equations utilized for the computation of geochemical indexes are reported in the following table:

Parameter	Equation
Total Iron as FeO (FeO _{tot})	$FeO_{tot} = FeO + 0.9 \cdot Fe_2O_3$
Larsen Index	$LarsenIndex = (1/3) \cdot SiO_2 + K_2O - MgO - CaO - FeO_{tot}$
Solidification Index (S.I.)	$S.I. = 100 \cdot \frac{MgO}{Na_2O + K_2O + FeO_{tot} + MgO}$
Magnesium Number (Mg#)	$Mg \#= 100 \cdot \frac{Mg}{Mg + Fe^{2+}}$
Alumina Saturation Index (ASI)	$ASI = molar \left(\frac{Al_2O_3}{Na_2O + K_2O + CaO} \right)$
Fe-Mg molecular ratio (Fe/Mg)	$Fe/Mg = \frac{FeO_{tot}}{MgO}$
Molar conversion	$MolarConversion = \frac{oxide_wt\%}{MolecularWeight}$

Additional features of Petrograph are the filter options; filters are useful when the user works with a large database containing heterogeneous analysis and he/she wants to plot only samples having peculiar characteristics. For example he/she can introduce a filter that allow the program to plot only that samples with a content of SiO_2 less then 50% wt. Petrograph will exclude automatically form the diagrams all the samples with a content of SiO_2 higher than 50% wt.

EXAMPLES

1 Import file and make a plot

In this example an Excel file will be imported and then a binary plot will be developed. Before importing an Excel file the user have to be sure that the spreadsheet is arranged in the correct way. To arrange correctly on Excel worksheet refer to paragraph 2.2 in the Main Features Section. The file Gede2001.xls (see the examples folder) can be used as an example and it can be imported with no changes.

To import the Gede2001.xls, select the "Import – file Excel (.XLS)" option from the file menu (Figure 14).

File Plot	ira V	philipping and a second s
Open Import))	File Excel (XLS)
Save		file IgpetWin (.ROC)
Exit		

Figure 14

Once the file is loaded, the "Data Table" will appear (Figure 15). Within the "Data Table" it is possible to change the symbol of each sample by selecting the relative cell in column "Symbol" and clicking the selected symbol lower part of the table. To change the colour of the sample proceed as before but act on the "Colour" column.

	Symbol	Color	Plot (0-1)	Si02	TiO2	AI203	Fe203	Fe
GDCS1	1	1	1	47.5	1.89	14.4	6.64	4.6
GD65	1	1	1	48.19	2.01	16.9	3.14	7.0
GD79	1	1	1	49.91	1.94	15.72	10.57	•
GD3	1	1	1	49.95	1.86	16.3	4.68	5.1
GD80A	1	1	1	50.04	1.81	16.5	9.46	0.3
GD80B	1	1	1	50.11	1.9	16.56	8.78	0.8
GD80C	1	1	1	50.2	1.83	16.54	5.02	4.1
GD83A	2	1	1	50.68	2.03	16.12	10.56	
GD83D	2	1	1	50.73	1.96	16.68	8.17	2.1
GD83C	2	1	1	51.08	2.08	16.48	8.61	1.8
GD66	2	1	1	51.21	1.87	18.15	6.27	3.1
GD83E	2	1	1	51.61	1.94	16.52	9.98	+
GD64	1	1	1	51.65	2.15	16.98	7.43	2.8
GD58	2	1	1	51.89	1.61	18.95	6.2	2.8
GD83F	2	1	1	51.89	1.84	16.56	10.58	
GD83I	2	1	1	52.14	1.79	17.78	9.59	-
GD57	2	1	1	52.38	1.69	18	5.54	3.4
GD83L	2	1	1	52.39	1.97	16.61	10.25	-
<[]				hierorisco.	- Parate -	heteroexes.	d incluin a	E.
Symbol (column 1) ■ 1 □ 2 △ 5 ▽ 6 # ◇ 9 × 10 -	3 ○ 4 7 + 8 11 ⊠ 12		Image: Provide the contract of the contract o	2	3 1 7 1	4 8 12	Double click to o concentration v Rigth click for o Hide	hange alues ptions

Figure 15

To make a binary plot, select the option "Binary plot" from the "Plot" menu (Figure 16) and the "Binary Plot Windows" will appear (Figure 17).

File	Plot Windows	2	
È	Binary Plot		N 🖾 🗉 🗵 💷 🗖 🌆 🕄
	Spider	•	
	Diagram Legend		



Binary Plot	×
X:	• LIN
Y:	• LIN
Graph Characteristic Graph Dim. (pixel) Width 500 Height 300	Symbol Dim Med Symbol Width
Operation Cancel	Plot (SpaceBarr)



Select the elements to be plotted by clicking the buttons and then create the diagram by clicking the "Plot(spacebar)" button. For example, selecting "Rb" for the x axis and "Sr" for the y axis the plot displayed in Figure 18 will be generated.



Figure 18

To adjust the x and y axes properties, make a double click on the graph and the windows displayed in Figure 19 will appear.





Replacing the minimum value for Rb and Sr with 0 and putting in the step interval 20 and 50 for Rb and Sr respectively a more readable diagram can be genetated (Figure 20)



Figure 20

2 Make a REE spider

To make a REE spider select the "Spider – REE" option from the "Plot" menu (Figure 21).





The "REE spider window" (Figure 22) will appear. This window allows to select the samples (max

50) to be plotted by clicking the button . Only samples with Eu analysed can be selected.

Ments Ce 68 La Sm Ho Ce B Fr Ce B Fr Md Fr 112 Nd Fr 11 Fr 11 Fr Fr 2 Tm No Th 03 Fr 2 Tm Md So Go So Go Go So Go Go So Go			La	.33	Contraction of the local division of the loc			
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Pm Dy Lu Instruct all Eu 069 Sc of MACC importance Control - Huadia et al (1998)	Nd TD Y	b	Sm	.181	1947		Add all	
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carafas). Carcen Lu 034	SpareFlar)	IOC EL	Lu	.034				

Figure 22

To generate the diagram (Figure 23) click the button "Plot(spacebar)" in the "REE spider Windows".



Figure 23

3 Make a Model for Major Elements

In this paragraph we show an example for the Mass Balance computation. In particular we reproduce the original example proposed by Stormer and Nichols in their paper published on Computer and Geosciences on 1978. The StormerNichols1978.xls file is stored in the example folders and it can be imported as described in the first example. To perform a Mass Balance computation select the "Mass Balance" option from the "Windows" menu (Figure 24) or click the button Σ from the control bar; as result, a blank "Mass Balance windows" will appear (Figure 25).



Figure 24

lect Oxides Sele	ct Magmas	Select Phase	es	
Α				
				*
				•

Figure 25

Now select oxides that will be utilized for the computation by clicking on the button with label "select oxides" in the "Mass Balace Window"; the windows displayed in Figure 25 will appear.

des				
SiO2	TiO2	AI2O3	FeOtot	MnO
MgO	CaO	Na2O	K20	P205
Clear	All	Select A		SpBar)



By observing oxides present in the imported database we see that P2O5 is lacking and therefore we unselect it. Selected oxides appear as green while the unselected oxides are red. In practice, to activate an unselect an oxide, click on it an it will change from red to green. To continue click on "OK (SpBar)". Now selected oxides will appear in the "Mass Balance windows" (Figure 27).

Mass Balan	ice: after Stormer &	Nicholls, 19
FINPUT D	ATA	
	Select Oxides	Select Ma
Si02		
Ti02		
AI203		
FeOtot		
MnO		
MgO		
CaO		
Na20		
K20		
TOT		

Figure 27

The initial and the final magma can be selected (Figure 28) by clicking the button with the label "Select Magmas" in the "Mass Balance Window".

nitial Magma	Final Magma
Select from Samples	Select from Samples
Open file	Open file

Figure 28

Clicking on "Select from Samples" a list for the available samples will appear and the choice can be performed by clicking on the selected sample. To repeat the example of Stormer and Nichols (1978), select the sample "RCB-153" as initial Magma, "RMD-277" as final magma and click the button "OK (Spacebar)". The initial an the final magma analyses will appear on the "Mass Balance Windows" (Figure 29).

	Sele	ct Oxides	Select Magmas	Select Phases
	Initial Magma	Final Magma		
SiO2	48.35	67.04		
TiO2	1.39	0.43		
AI203	15	15.6		
FeOtot	12.24	2.54		
MnO	0.19	0.04		
MgO	8.94	1.29		
CaO	8.93	3.96		
Na20	3.2	4.61		
K20	0.92	2.36		
гот	99,16	97.87		



Now it is necessary to select the phases that will be subtracted from the initial magma to reach the final magma. To do it, click the button "Select Phases" and the window displayed in Figure 30 will appear.



Figure 30

To select a phase click on a red button, when all the phases of interest are activated click on the button "OK (Spacebar). In this case we select the Amphibole "HB199" plus Albite (AB) and Anortite (AN) phases as Stormer and Nicholls did in their original paper. Now all the element required to perform the Mass Balance are ready; to start the computation click on the button "Calculate (Spacebar)". Results (Figure 31) will be displayed on the lower part of the "Mass Balance Window" in the same way of the original paper by Stormer and Nichols. Results can be also copied in the clipboard and successively pasted in another application like, such as, MS Excel (Figure 32).

	Sel	ect Oxides		Sele	ct Magma	s Select P	tias	es :	
	Initial Magma	Final Magma	HE	1199	AB	AN			
SiO2	40.35	\$7.04	15.4	4	68.74	43.19			
Ti02	1.39	0.43	3.8		0	0			
AI203	15	15.6	\$2.1	1	13.44	16.65			
FeOtot	12.24	2.54	\$8.5	5	0	0			
MnO	0.19	0.04	0.2		0	0			
MgO	0.54	1.29	54.5	ł	0	0			
CaO	8.92	0.96	12.2	1	0	20.16			
Na20	3.2	4.61	1.4		11.82	0			
K20	0.92	2.14	0		0	0			
TOT	Date no.	97.87	201.4	4	2100	8100			
OUTPU	T DAT/								
OUTPU SUM OF	T DAT/	THE SQUAF	RES	OF TH	æ	RESIDUALS		1.5115	2
OUTPU SUM OF PHASE	T DAT/	THE SQUAF	AES S	OF TH	HE UNT AS	RESIDUALS AMOUNT AS	AM	1.5115 IOUNT AS	
OUTPU SUM OF PHASE NAME	T DAT	THE SQUAF	nes s	OF TH AMOUNT 3	HE UNT AS	RESIDUALS AMOUNT AS WT 3 OF	AM	1.5115 IOUNT AS 1.3: OF	
OUTPU SUM OF PHASE NAME	T DAT/	THE SQUAF AMOUNT A WT % OF INIT, MAGH	PES S	OF TH AMOU WT 3 ALL F	HE UNT AS LOF HASES	RESIDUALS AMOUNT AS WT 3: OF ADDED PHS	AM W1 SU	1.5115 IOUNT AS I. X: OF BTRD PHS.	
OUTPU SUM OF PHASE NAME HB199	T DAT/	THE SQUAF AMOUNT A WT 2: OF INIT. MAGH	RES S M 58.2	OF TH AMOU WT 3 ALL F	HE UNT AS LOF HASES 82.92	RESIDUALS AMOUNT AS WT % OF ADDED PHS.	AM W1 SU	1.5115 IOUNT AS 1.3; OF BTRD PHS. 82; 92	
OUTPU SUM OF PHASE NAME HB199 AB	T DAT/	THE SQUAF AMOUNT A WT 2: OF INIT. MAGH	RES S 58.2 8.41	OF TH AMOU WT 3 ALL F	HE UNT AS OF HASES 82.92 11.98	RESIDUALS AMOUNT AS WT & OF ADOED PHS.	AM W1 SU	1.5115 IOUNT AS 1.3: OF BTRD PHS. 82: 92 11.90	
OUTPU SUM OF PHASE NAME HB199 AB AN	T DAT/	THE SQUAF AMOUNT A WT 2: OF INIT. MAGH 4 4	RES S 58 2 8.41 3 58	OF TH AMOU WT.3 ALL F	HE UNT AS COF HASES 82.92 11.98 5.1	RESIDUALS AMOUNT AS WT & OF ADDED PHS 0 0 0	AM W7 SU	1.5115 IOUNT AS 1.3: OF BTRD PHS. 82: 52 11.90 5.1	
OUTPU SUM OF PHASE NAME HB199 AB AN	T DAT	THE SQUAF AMOUNT A WT X OF INIT. MAGM 4 4 5	RES S 58.2 8.41 3.58	OF TH AMOU WT.3 ALL F	HE UNT AS COF HASES 82.92 11.98 5.1	RESIDUALS AMOUNT AS WT % OF ADDED PHS	AM W/T SU	1.5115 IOUNT AS 1 % OF BTRD PHS. 82.52 11.98 5.1	2
OUTPU SUM OF PHASE NAME HB199 AB AN TOTAL I	T DAT	THE SQUAF AMOUNT A WT X OF INIT MAGM	RES S 58.2 8.41 3.58	OF TH AMOU WT 3 ALL F	HE LINT AS OF HASES 82.92 11.98 5.1 MA	RESIDUALS AMOUNT AS WT 3: OF ADDED PHS 0 0 0	AM W1 SU	1.5115 IOUNT AS 1.3; OF BTRD PHS. 82:92 11.99 5.1 70.18	د د لا

Figure 31

RECAL.	ANALYSES	(WT.%)	TO 100%		
OXIDE	INIT	FINAL	HB199	AB	AN
SiO2	48.75958	68.49903	35.98	68.74	43.19
TiO2	1.401775	0.4393583	3.86	0	a
AI2O3	15.12707	15.93951	12.3	19.44	36.65
FeOtot	12.34369	2.595279	18.8	0	a
MnO	0.1916095	4.09E-02	0.2	0	0
MgO	9.015732	1.318075	15.04	0	a
CaO	9.005648	4.046184	12.4	0	20.16
Na2O	3.227108	4.71033	1.42	11.82	a
K2O	0.9277935	2.411362	0	0	0
тот	100	100	100	100	100
RESULTS					
	BULK COMP.	OBS.DIFF.	CALC.DIFF.	OBSCALC.	
	OR ADDED OR	BETWEEN	BETWEEN	RESIDUALS	
OXIDE	SUBTR.MATL.	MAGMAS	MAGMAS		
SiO2	40.268	19.739	19.813	-0.074	
TiO2	3.202	-0.962	-1.939	0.977	
AI2O3	14.394	0.812	1.085	-0.272	
FeOtot	15.59	-9.748	-9.12	-0.628	
MnO	0.169	-0.151	-0.09	-0.061	
MgO	12.472	-7.698	-7.828	0.131	
CaO	11.309	-4.959	-5.097	0.138	
Na2O	2.596	1.483	1.484	-0.001	
K20	0	1.484	1.692	-0.209	
			TOTAL	0	
SUM OF	THE SQUARES	OF THE	RESIDUALS	1.5115	
PHASE	AMOUNT AS	AMOUNT AS	AMOUNT AS	AMOUNT AS	
NAME	WT.% OF	WT.% OF	WT.% OF	WT.% OF	
	INIT. MAGMA	ALL PHASES	ADDED PHS.	SUBTRD.PHS.	
HB199	-58.2	82.92	0	82.92	
AB	-8.41	11.98	0	11.98	
AN	-3.58	5.1	0	5.1	
TOTAL REI	TO INITIAL	MAGMA	0	70.18	

Figure 32

4 Make a Trace Elements model

Trace elements models can be performed by Petrograph directly on binary diagrams. In this example we develop a Fractional Crystallization model for an incompatible element against a compatible one (see Peccerillo et al., 2003 for details). We first create a binary plot on the file Gede2001.xls as described in the first example. In particular we set in the x axis a compatible element like Vanadium (V) while in the y axis we set an incompatible element like Zirconium (Zr). To develop a trace element model, click the right button on the diagram and select the option "Insert Model – Models Generator" from the cascade menu (Figure 33).



Figure 33



Models			
MODEL:	FC		
D for V D for Zr	4 0.1	F tmelt fraction 8-1) From 0.1 To 1 Step 0.1	Symbol (click to sel.) 1 2 0 3 0 4 4 5 7 6 8 7 + 8 0 9
		Patent CB select s Select CO on graph	Symbol Mr Color Symbol
			Line 1 S Width Color
			Cancel
			Ok (SpaceBar)



Select the "FC" model from the Cascade list in the upper part of the window, insert values for the bulk partition coefficient for V (D_V =4) and Zr (D_{Zr} =0.1) and select GD65 as "Parent magma" (CO). It is possible to select the "Parent" magma in two ways: (i) by selecting it from the cascade list with the label "Parent CO" or (ii) by clicking the "Select CO on graph" button and selecting the parent magma directly on the graph with a click on a sample. For this example we select the sample "GD65" as parent magma. To plot the model (Figure 35) on the graph click the "OK (Spacebar)" button.



Figure 35

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CREDITS

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