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Short note

GeoPlot: An Excel VBA program for geochemical data plotting ☆

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1. Introduction

Microsoft Excel™ is a spreadsheet application widely used by geochemists for data storage and manipulation. It has limited functionality for geochemists as only manual data organization and basic *X–Y* plots are available for data interpretation. Consequently some software packages such as MinPet (Richard, 1997), Igpet (Carr, 1995), Newpet (Clarke, 1993) and PETROGRAPH (Petrelli, 2003) have been developed for better data visualization and interpretation. However, all these programs only have access to the plot functionalities that are not directly linked to a spreadsheet. The programs require the data set in the Excel format to be imported or converted to an external file with certain formats, and this procedure has to be repeated every time the data set is updated. In addition, these programs have many discrimination diagrams but users cannot customize or add new ones. Although several previous Excel macro programs are capable of plotting *X–Y* plots and triangular plots (e.g., Sidder, 1994; Christie and Langmuir, 1994; Marshall, 1996), they cannot meet the need of today's geochemists using an advanced computer system. The program PetroPlot of Su et al. (2003) has the plotting functions of multi-series *X–Y* plots and spider diagrams. However, it cannot deal with the commonly used triangular plots and discrimination diagrams. This paper presents here a new VBA program named "GeoPlot" for geochemical data plotting in Microsoft Excel™.

GeoPlot has the following major plotting functions: *X–Y* plot and triangular plot, spider diagram and discrimination diagram, and related functions such as calculating formulas and CIPW norm. Moreover, GeoPlot also contains many discrimination diagrams and normalization values used for spider diagrams. Using GeoPlot, users can also manually add new normalization values and new discrimination diagrams into the program. GeoPlot provides a menu and a toolbar in Excel for allowing easy management of these functions. The geochemical data processed by GeoPlot in the user's data worksheet should be arranged in one simple format, allocating the element names in the first column and sample names in the first row and every element value of a sample in the corresponding column. The manual for GeoPlot, which contains detailed user guide information, is included in the "Help" file.

2. GeoPlot functions

2.1. *X–Y* plot

Based on the selected element names or formula strings entered in the "*XY* plot dialog box" (Fig. 1), the

☆Code available from server at http://www.iamg.org/CGEditor/index.htm.

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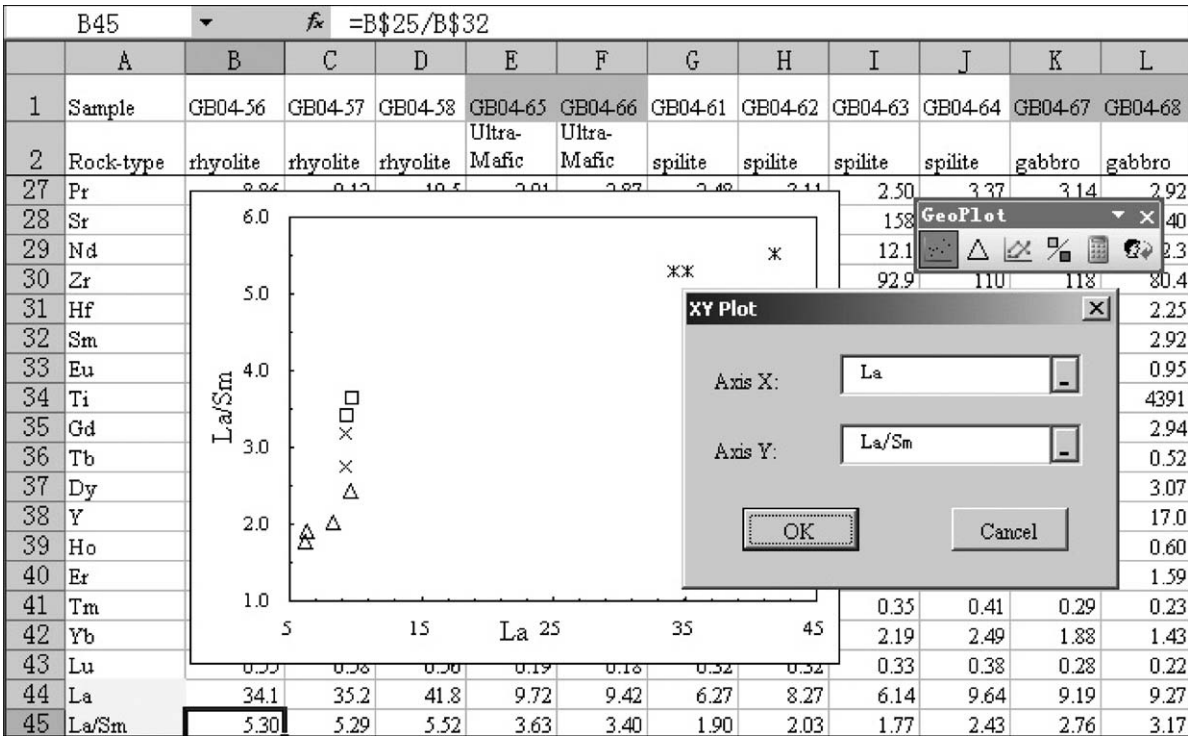
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program can confirm the *X*- and *Y*-axis formula strings. Using a string processing technique the program can distinguish the element names among the calculation operators in the formula strings and finds their row addresses in the data worksheet (see Section 2.5 for details). GeoPlot further replaces the element names in the formula strings with their corresponding row addresses in the data worksheet, generating the formulas compatible with Excel. The program makes two blank rows, which are just below the data arrays in the data worksheet, equal to the replaced formulas for *X*- and *Y*-axes. By adding the above two rows of data into an Excel *XY* scatter chart, the program can produce an *X*–*Y* plot. If the samples are subdivided into groups or series (see Section 3.1 for details), GeoPlot subdivides the two rows of data into the same series and adds them into an Excel *XY* scatter chart one by one to get a multi-series *XY* plot. For example, to make the La/Sm–La plot, geochemists may select the element names of "La" and "Sm" in their data worksheet and modify them to form the correct *X*- and *Y*-axis formulas of "La" and "La/Sm" in the "*XY* plot dialog box" (Fig. 1). After clicking the "OK" button, users automatically obtain the La/Sm–La plot. Users can manually change the axis scale from the default linear scale to the logarithmic scale in the *X*–*Y* plot if necessary.

2.2. Triangular plot

Although Excel is unable to make a triangular plot directly, this can be achieved by using an Excel's *XY* scatter plot as described by Christie and Langmuir (1994) and Marshall (1996). To plot a triangular chart, the raw data for *A*, *B* and *C* apexes (counterclockwise from the left apex of the triangle) must be converted into the percent data for A', B' and C' according to their proportion. Then using the formulas $x = B' + C'/2$ and $y = C' * 0.866$ (the height of an equilateral triangle is equal to its width multiplied by $\sin 60^\circ \approx 0.866$), the program can compute the coordinates for an Excel *XY* scatter chart. The above process is incorporated into the formulas acceptable to Excel (e.g., the "*fx*" bar, top of Fig. 2, shows the resulting formula of "*y*" for the "triangular plot"). The method of structuring the above formula is the same as that for processing an *X*–*Y* plot. After structuring the formulas, the program makes two blank rows, which is just below the data arrays in the data worksheet, equal to the formulas for *X*- and *Y*-axes. After adding the two rows of data to an Excel *XY* scatter chart, the program produces an *X*–*Y* plot. If the samples are subdivided into some series, the processing is the same as that in the *X*–*Y* plot. Finally, the triangular plot is obtained after replacing the axes of the *X*–*Y* plot with triangular sides.



	A	B	C	D	E	F	G	H	I	J	K	L
1	Sample	GB04-56	GB04-57	GB04-58	GB04-65	GB04-66	GB04-61	GB04-62	GB04-63	GB04-64	GB04-67	GB04-68
2	Rock-type	rhyolite	rhyolite	rhyolite	Ultra-Mafic	Ultra-Mafic	spilite	spilite	spilite	spilite	gabbro	gabbro
27	Pr								2.50	3.37	3.14	2.92
28	Sr								158			40
29	Nd								12.1			2.3
30	Zr								92.9	110	118	80.4
31	Hf											2.25
32	Sm											2.92
33	Eu											0.95
34	Ti											4391
35	Gd											2.94
36	Tb											0.52
37	Dy											3.07
38	Y											17.0
39	Ho											0.60
40	Er											1.59
41	Tm								0.35	0.41	0.29	0.23
42	Yb								2.19	2.49	1.88	1.43
43	Lu								0.33	0.38	0.28	0.22
44	La	34.1	35.2	41.8	9.72	9.42	6.27	8.27	6.14	9.64	9.19	9.27
45	La/Sm	5.30	5.29	5.52	3.63	3.40	1.90	2.03	1.77	2.43	2.76	3.17

Fig. 1. Dialog box of *X*–*Y* plot and resultant La/Sm–La scatter plot.

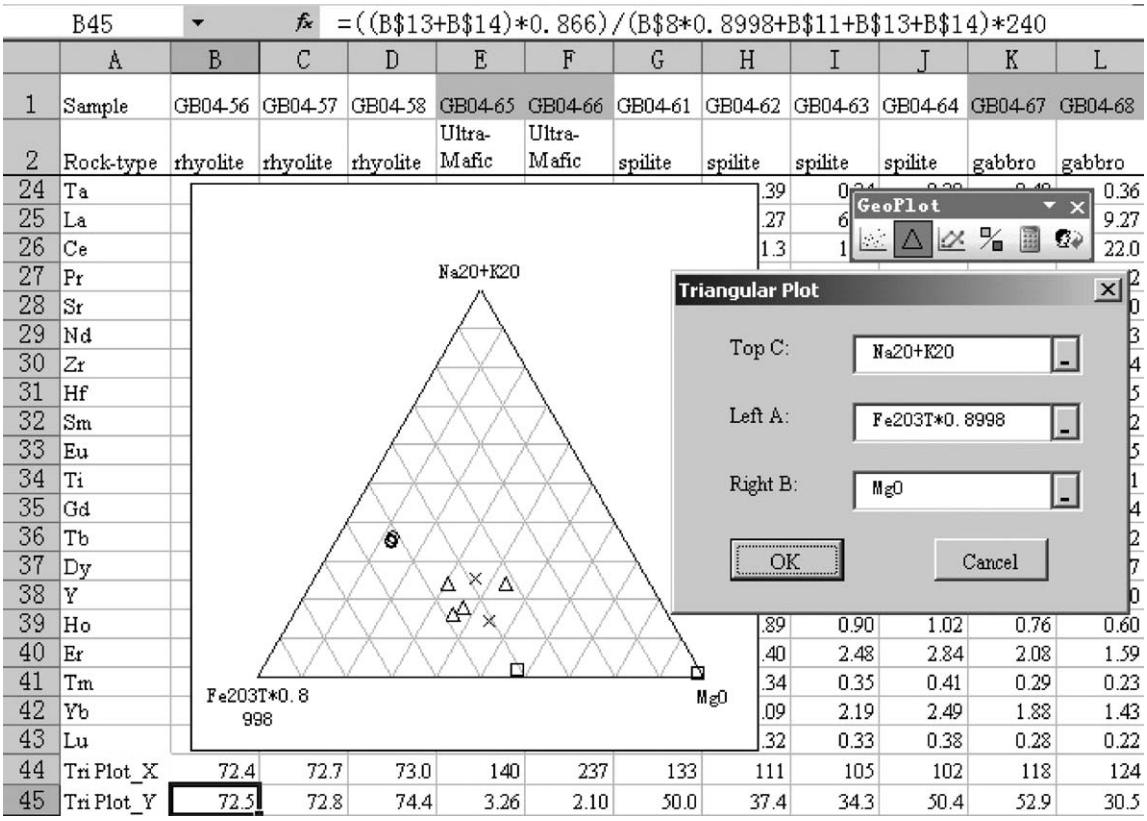


Fig. 2. Dialog box of triangular plot and resultant AFM triangular plot.

2.3. Spider diagram

GeoPlot can automatically plot REE spidergrams and trace element spidergrams. The program provides many selections of the normalization values from GeoPlot's internal workbook. At the same time, GeoPlot provides three reference series for selection (see Fig. 3). The user should select one sequence of normalization values and optionally select the three reference series. GeoPlot can then locate every element of the selected sequence of normalization values in the data worksheet and divides the corresponding element data by the normalization values. The program uses an Excel's line chart to plot the spidergram with the calculated data. Finally, the resultant data and spidergram are provided in a new worksheet (Fig. 4).

2.4. Discrimination diagram

Geochemists often use discrimination diagrams to determine rock classification, petrogenesis and tectonic setting, in which the rock formed. It is some times difficult to plot these discrimination diagrams without using software, such as MinPet (Richard, 1997). GeoPlot contains many discrimination diagrams consistent with the built-in diagrams within MinPet, and users can also add new discrimination diagrams into GeoPlot.

There are two categories of diagrams, i.e. the X–Y plot (e.g., Fig. 5) and triangular plot (e.g., Fig. 6), in the discrimination diagrams. GeoPlot firstly draws the discrimination lines and labels using the specification data from GeoPlot's internal workbook in an Excel XY scatter chart. Then GeoPlot constructs the formulas for the plotted data. The method of the formulation is the same as that in processing the X–Y plot or triangular plot. Finally, the program can plot the resulting data into the discrimination diagram as an X–Y plot or triangular plot. If the samples are subdivided into some series, the processing is also the same as that in the X–Y plot.

2.5. Calculating formulas

It is the fundamental function of GeoPlot to allow the calculation of formula strings. In the process of structuring a formula acceptable to Excel, GeoPlot uses the calculation operators and the seven commonly used functions of *Sqrt, Ln, Log*10*, Log, Exp, Power* and *Sum*. Using the function of "IsNumeric" in Excel VBA, the

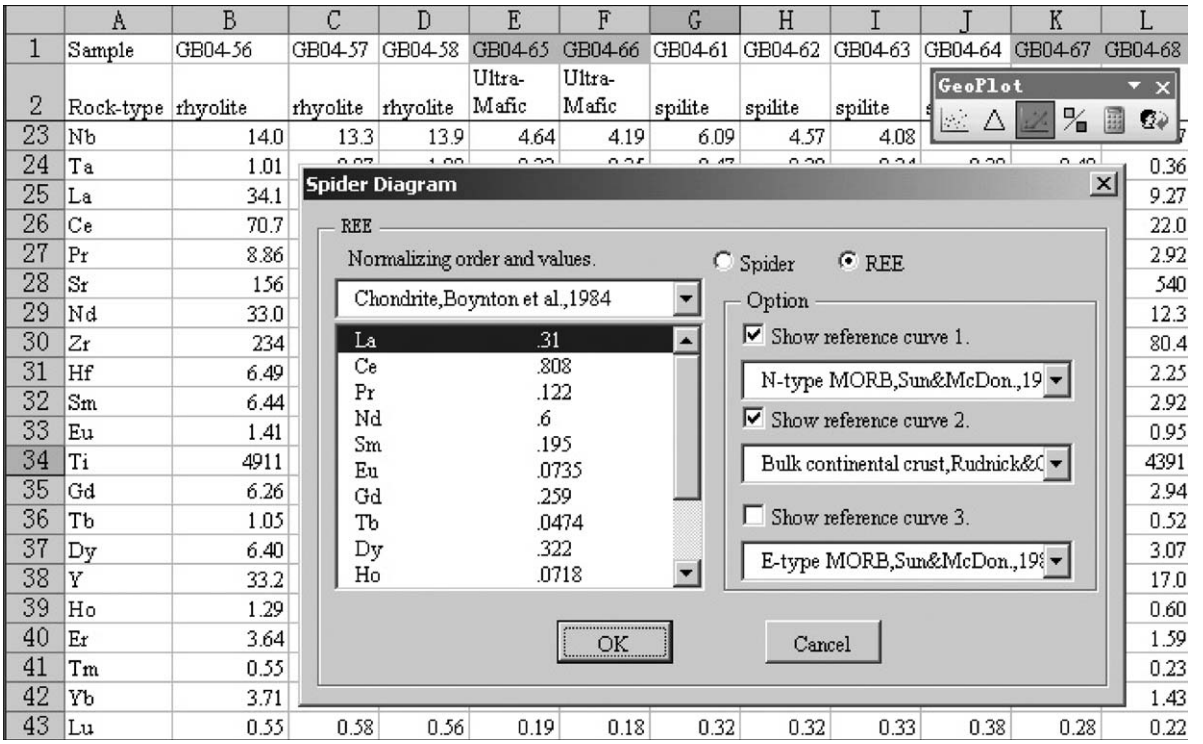


Fig. 3. Dialog box of REE distribution diagram.

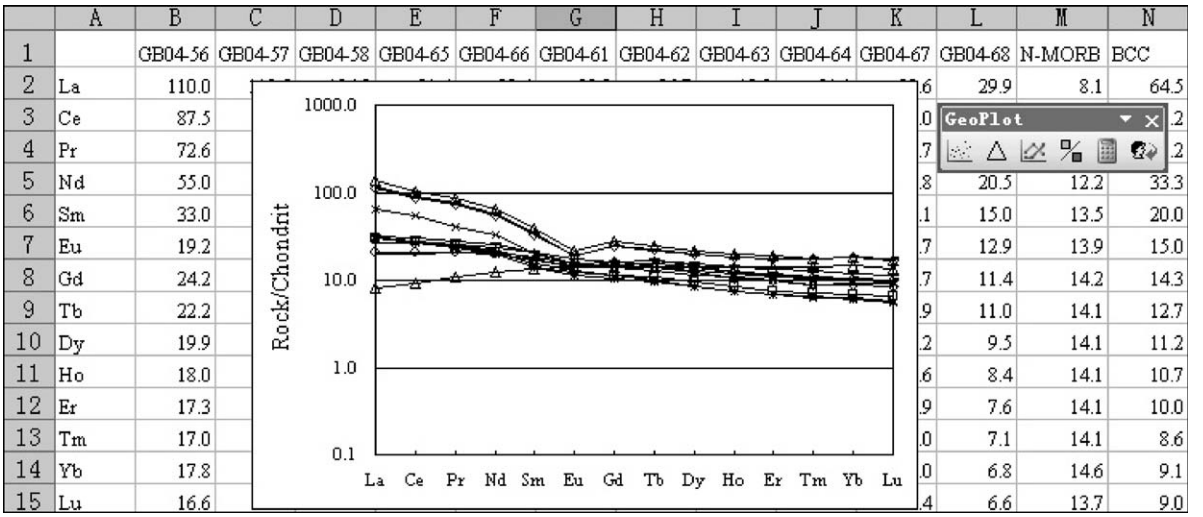
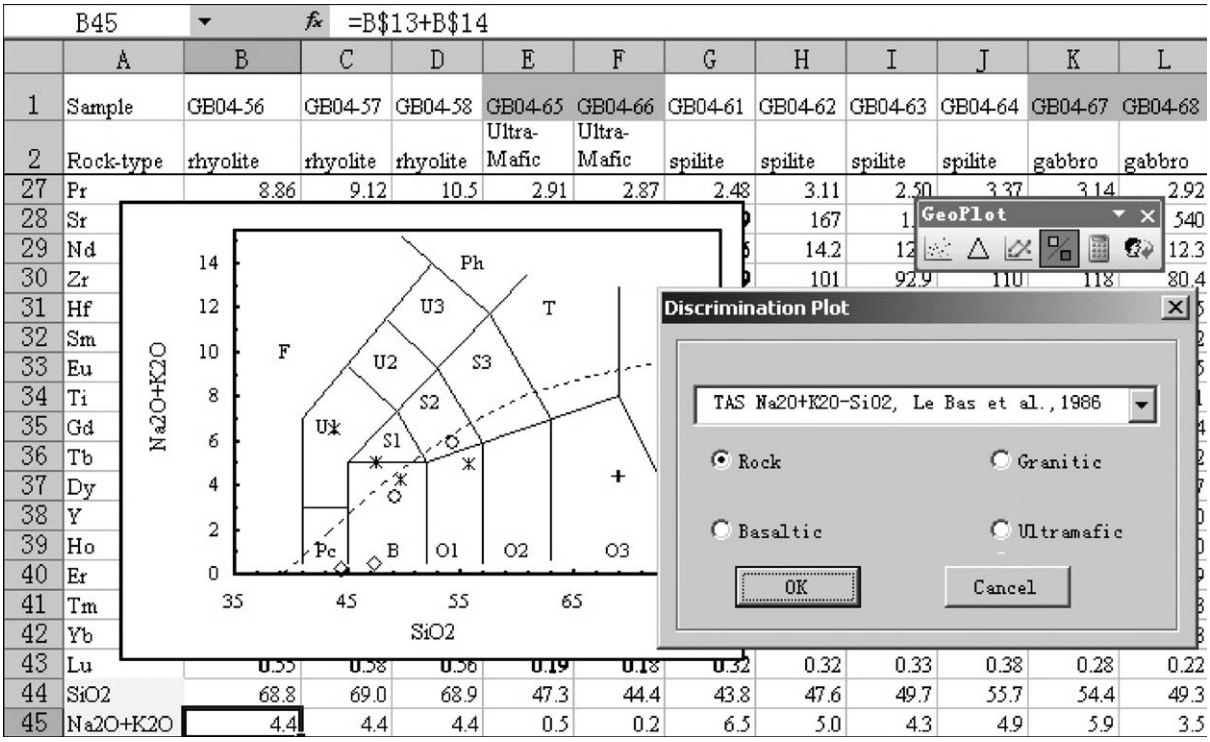


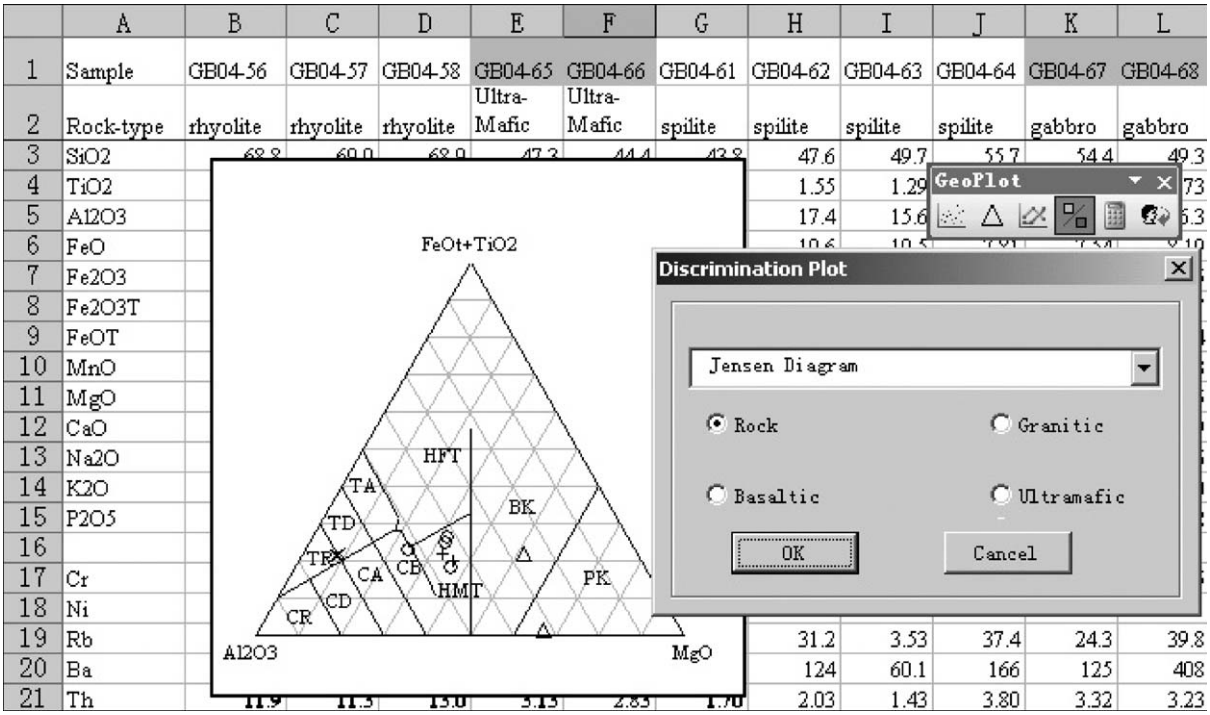
Fig. 4. Chondrite-normalized data and resultant REE distribution diagram.

program can identify each group of characters, which is separated by the calculation operators in the formula string, as either an alphabetic word or numeric value. Moreover, GeoPlot can further identify whether each alphabetic word is a function name (e.g., *Sqrt*) or an element name (e.g., SiO_2). The program then locates these identified element names in a user's data worksheet and replaces these element names in the formula string with their corresponding row addresses in the data worksheet. A formula, which can be processed by Excel, is obtained after the replacement of the element names (e.g., Fig. 7 shows the resulting formula in the "*fx*" bar



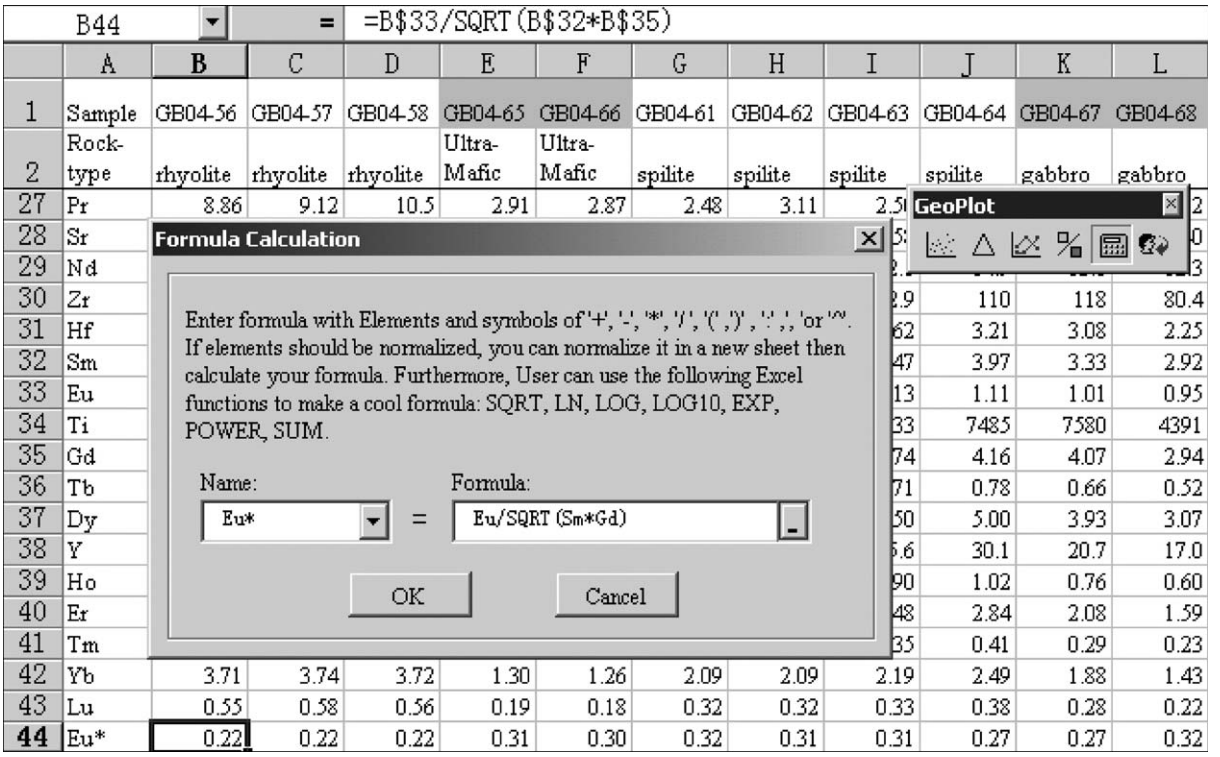
	A	B	C	D	E	F	G	H	I	J	K	L
1	Sample	GB04-56	GB04-57	GB04-58	GB04-65	GB04-66	GB04-61	GB04-62	GB04-63	GB04-64	GB04-67	GB04-68
2	Rock-type	rhyolite	rhyolite	rhyolite	Ultra-Mafic	Ultra-Mafic	spilite	spilite	spilite	spilite	gabbro	gabbro
27	Pr	8.86	9.12	10.5	2.91	2.87	2.48	3.11	2.50	3.37	3.14	2.92
28	Sr							167	1			540
29	Nd							14.2	12			12.3
30	Zr							101	92.9	110	118	80.4
31	Hf											
32	Sm											
33	Eu											
34	Ti											
35	Gd											
36	Tb											
37	Dy											
38	Y											
39	Ho											
40	Er											
41	Tm											
42	Yb											
43	Lu	0.55	0.58	0.56	0.19	0.18	0.32	0.32	0.33	0.38	0.28	0.22
44	SiO2	68.8	69.0	68.9	47.3	44.4	43.8	47.6	49.7	55.7	54.4	49.3
45	Na2O+K2O	4.4	4.4	4.4	0.5	0.2	6.5	5.0	4.3	4.9	5.9	3.5

Fig. 5. Dialog box of discrimination plot and TAS diagram.



	A	B	C	D	E	F	G	H	I	J	K	L
1	Sample	GB04-56	GB04-57	GB04-58	GB04-65	GB04-66	GB04-61	GB04-62	GB04-63	GB04-64	GB04-67	GB04-68
2	Rock-type	rhyolite	rhyolite	rhyolite	Ultra-Mafic	Ultra-Mafic	spilite	spilite	spilite	spilite	gabbro	gabbro
3	SiO2							47.6	49.7	55.7	54.4	49.3
4	TiO2							1.55	1.29			73
5	Al2O3							17.4	15.6			6.3
6	FeO											
7	Fe2O3											
8	Fe2O3T											
9	FeOT											
10	MnO											
11	MgO											
12	CaO											
13	Na2O											
14	K2O											
15	P2O5											
16												
17	Cr											
18	Ni											
19	Rb							31.2	3.53	37.4	24.3	39.8
20	Ba							124	60.1	166	125	408
21	Th	11.9	11.3	13.0	3.13	2.83	1.70	2.03	1.43	3.80	3.32	3.23

Fig. 6. Dialog box of discrimination plot and Jensen diagram.



	A	B	C	D	E	F	G	H	I	J	K	L
1	Sample	GB04-56	GB04-57	GB04-58	GB04-65	GB04-66	GB04-61	GB04-62	GB04-63	GB04-64	GB04-67	GB04-68
2	Rock-type	rhyolite	rhyolite	rhyolite	Ultra-Mafic	Ultra-Mafic	spilite	spilite	spilite	spilite	gabbro	gabbro
27	Pr	8.86	9.12	10.5	2.91	2.87	2.48	3.11	2.5			2
28	Sr								5			0
29	Nd											3
30	Zr								2.9	110	118	80.4
31	Hf								62	3.21	3.08	2.25
32	Sm								47	3.97	3.33	2.92
33	Eu								13	1.11	1.01	0.95
34	Ti								33	7485	7580	4391
35	Gd								74	4.16	4.07	2.94
36	Tb								71	0.78	0.66	0.52
37	Dy								50	5.00	3.93	3.07
38	Y								5.6	30.1	20.7	17.0
39	Ho								90	1.02	0.76	0.60
40	Er								48	2.84	2.08	1.59
41	Tm								35	0.41	0.29	0.23
42	Yb	3.71	3.74	3.72	1.30	1.26	2.09	2.09	2.19	2.49	1.88	1.43
43	Lu	0.55	0.58	0.56	0.19	0.18	0.32	0.32	0.33	0.38	0.28	0.22
44	Eu*	0.22	0.22	0.22	0.31	0.30	0.32	0.31	0.31	0.27	0.27	0.32

Fig. 7. Dialog box of formula calculation.

and the original formula string in the dialog box). Finally, the program makes a blank row, which is just below the data array in the user's data worksheet, equal to the evaluation of the formula.

2.6. CIPW norm

As we know, the CIPW norm is used to calculate the idealized mineral assemblage of an igneous rock. Some programs can run the CIPW norm calculation, such as MinPet, Igpet, Newpet, PETROGRAPH and SINCLAS (Verma et al., 2002). The SINCLAS program is the best for taking into account the minor chemical constituents in calculations. All these programs do not run in the Excel environment.

There is a spreadsheet program capable of running CIPW norm[1] but it only calculates one sample each time. In contrast, GeoPlot was designed to calculate as many as 255 samples each time in a data worksheet. The CIPW norm in GeoPlot is performed using the calculation scheme of Best (2003). GeoPlot uses eleven major oxides for common igneous rocks to produce normative minerals: SiO_2, TO_2, Al_2O_3, Fe_2O_3, FeO, MnO, MgO, CaO, Na_2O, K_2O and P_2O_5. The results of this CIPW norm are consistent with that of SINCLAS program, both using the same major oxides data.

[1]This program was written by Kurt Hollocher, Geology Department, Union College, Schenectady, NY 12308, hollochk@union.edu.

3. Customization

3.1. Data series

Geochemists often analyze many samples that are subdivided into groups or series. The data of each series must be allocated into continuous columns in an Excel worksheet. The background colors of the cells in the first row for a series, which is used to allocate the sample names, must be uniform. In the *X–Y* plot, triangular plot or discrimination diagram, data are acquiescently divided into series. Each series has a uniform symbol that is randomly given by Excel (e.g., Fig. 5). Users can change the symbols of the series as they commonly do on an Excel *XY* scatter chart.

3.2. Using the "User Database.xls"

A user can use the file of "User Database.xls" to customize GeoPlot. Its structure is different from GeoPlot's internal workbook because there is an additional "*Reference*" worksheet in "User Database.xls". "*Reference*" worksheet has useful composition values, including the composition data of crust, mantle,

chondrite, MORB, OIB and some typical arc basalts. Users can manually add the new normalization values for spider diagrams and the specification data for a new discrimination diagram into this file in agreement with the already designed formats. The new customized data can be further added into GeoPlot's internal workbook by the "Database Manage" function in GeoPlot. Then users can plot their data using the new customized data in GeoPlot. In view of the limited length of the present paper, the details on the use of "User Database.xls" are included in GeoPlot's "Help" file.

4. Conclusion

GeoPlot provides the following plotting functions: X–Y plot, triangular plot, spider diagram and discrimination diagram, and related functions such as calculating formulas and CIPW norm. Users can add new normalization values for spider diagrams and the specification data of a new discrimination diagram into GeoPlot. This program has the advantage over the existing stand-alone plotting programs in that it allows data to be plotted and visualized easily in the same Excel environment, which geochemists often use to organize and valuate the data. In summary, GeoPlot provides a practical and simple solution for plotting geochemical data in Excel. The source codes are accessible to all users and can be modified for some special use.

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Appendix A. Electronic Supplementary Material

The online version of this article contains additional supplementary data. Please visit doi:10.1016/j.cageo.2005.07.005.

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