PERIODICO di MINERALOGIA
established in 1930

An International Journal of
Mineralogy, Crystallography, Geochemistry,
Ore Deposits, Petrology, Volcanology
and applied topics on Environment, Archaeometry and Cultural Heritage

Tetra-Plot: A Microsoft Excel spreadsheet to perform tetrahedral diagrams

Short Note

Ciro Cucciniello

Dipartimento di Scienze della Terra, dell'Ambiente e delle Risorse (DiSTAR), Università di Napoli Federico II, Via Mezzocannone 8, 80134 Napoli, Italy

ARTICLE INFO

Submitted: January 2016
Accepted: February 2016
Available on line: March 2016

Email: ciro.cucciniello@unina.it

DOI: 10.2451/2016PM625

How to cite this article:
Cucciniello C. (2016) Period. Mineral. 85, 115-119

ABSTRACT

Tetra-plot is a Microsoft Excel spreadsheet developed for the visualization of mineralogical, petrological and geochemical data in three dimensions. This program allows to normalize and plot a number of data on tetrahedral diagrams. The tetrahedron can be freely rotated in space. Tetra-Plot includes a set of functionalities that help users to manipulate data for 3D visualization.

Keywords: Geochemistry, Mineralogy, Petrology, Tetrahedron, Microsoft Excel®; Spreadsheet.

INTRODUCTION

Mineralogists, geochemists and petrologists commonly use binary, spider and ternary diagrams to represent mineral data, whole-rock geochemistry and phase relations of chemical systems. Interpretation of these data requires visualization of large data sets in multiple dimensions. For the study of phase systems or for the modeling of geochemical data, it may be useful to represent rock or mineral analyses in tetrahedral diagrams.

A number of computer programs have been developed to plot the data, such as TETRASEZ (Armienti, 1986), CSpace (Torres-Roldan et al., 2000), CMAS 3D (France et al., 2009), MetaRep (France and Nicolette, 2010), TetPlot (written by Frank S. Spear) and TetLab (written by Peter Appel). These programs run on programming language platforms such as FORTRAN, BASIC, JAVA and Cocoa (application programming interface for the OS X operating system). All these programs are useful, but often not simple to handle. To copy or import the data into these programs can be very time consuming and the charts should get reworked with graphics software before they can be used for presentations.

A simple spreadsheet for tetrahedral diagrams has been introduced by Shimura and Kemp (2015).

A new program is presented here "Tetra-Plot" a Microsoft Excel spreadsheet. It is a spreadsheet application allows to normalize and plot four different variables on tetrahedral diagrams. This spreadsheet has been designed to represent mineral and whole-rock geochemistry in igneous and metamorphic petrology. Tetra-Plot was developed using Excel® 2011 for Apple Macintosh. It should work with all Excel versions for Macintosh and PC running Windows XP, 7, 8 and 10, as well as Apache OpenOffice. This program is simple to handle and do not use VBA macros. It has a familiar user interface and data can be easily cut-and-pasted into the excel spreadsheet. Tetra-Plot can be downloaded at http://periodicodimineralogia.it/index.php/mineralogia/issue/view/30/showToc.

Compared to the spreadsheet of Shimura and Kemp (2015), Tetra-Plot:

1. Can plot the data also in a single triangle face of the tetrahedron
2. Can plot isotope data on tetrahedral diagrams
3. The tetrahedrons can rotate around all axes
4. The charts show automatically the apex-titles
5. The data can be easily selected using drop down menu

TETRA-PLOT SPREADSHEET

The Tetra-Plot spreadsheet consists of seven worksheets (Input data, Calculated data, Tetrahedron major elements, Tetrahedron trace elements, Tetrahedron isotopes, Tetrahedron CIPW and Note). The Input data and Calculated data worksheets contain the data entry and calculation area. Data can be imported from the clipboard or entered from the keyboard. By default, up to 200 data points can be plotted (see for example Figure 1). However, the user can increase the input data easily by adding more rows in the Input data worksheet and, then copying and pasting the formulas in the Calculated data worksheet. The Tetrahedron major elements, Tetrahedron trace elements, Tetrahedron isotopes and Tetrahedron CIPW worksheets contain tetrahedral diagrams. These diagrams are standard XY scatter graphs and can be modified to change parameters such as symbols, colours, size, line thickness. Each tetrahedral diagram contains different data series (major elements in wt%, trace elements in ppm, etc.). The list of data series is reported in the Calculated data worksheet. Any data sets can be plotted on a single tetrahedral diagram. Then, the tetrahedral diagrams can be copied to the clipboard and pasted into a suite of software for presentations.

The user should not delete any columns or rows containing the calculations crucial to the construction or movement of the tetrahedron.

TETRAHEDRAL PLOTS

To plot data into a tetrahedral diagram occur four steps: 1) build the tetrahedron; 2) collect raw data (e.g. whole-rock and mineral data) for the four variable of interest; 3) normalize the raw data; 4) plot the normalized data on the tetrahedral diagram.

The tetrahedron is constructed with four equilateral triangle faces and four vertices (named A, B, C and D; Figure 2). The coordinates of the vertices are: A (0.0; -57.7), B (0.0; 0.0), C (50.0; -28.9) and D (-50.0; -28.9). The apex represents the 100% of a component. The user can easily select each apex using the drop down menu (Figure 3) in the Calculated data worksheet. The apex titles will be automatically displayed on the diagram.

The raw data of the four apexes (A, B, C and D) must be changed into normalized data. The equations to do this are:

$$Y=((A\times 86.6025+B\times (28.8675))/((A+B+C+D)-28.8675)$$

$$X=(A\times 0+B\times 0+C\times 50+D\times (-50))/(A+B+C+D)$$

$$Z=B\times (-81.6497)/(A+B+C+D)$$

The equations to change the unnormalized data to

INSERT MAJOR, TRACE ELEMENT AND ISOTOPE VALUES HERE (BLUE FIELD)

READ ME

Sample name	Rock type	SiO_2	TiO_2	Al_2O_3	Fe_2O_3	FeO	MnO	MgO	CaO	Na_2O	K_2O	P_2O_5	SiO_2/10	TiO_2*10	Na_2O*10	K_2O*10	P_2O_5*10
L41	bsn	42.91	2.48	10.79	13.25		0.18	13.29	11.78	3.23	1.06	1.02	4.29	24.76	32.33	10.64	10.23
gh15	tph	45.88	4.07	15.04	11.79		0.12	8.45	10.78	1.73	1.34	0.80	4.59	40.72	17.33	13.41	7.96
gh14	bsn	43.16	3.62	13.62	14.26		0.17	7.47	13.62	2.26	1.13	0.69	4.32	36.22	22.62	11.31	6.94
L37	tph	46.05	3.35	12.63	11.49		0.20	5.29	14.77	3.00	2.34	0.88	4.61	33.47	29.99	23.40	8.79
LY 2B	ab	47.68	1.89	12.69	11.86		0.16	11.25	9.59	3.33	1.01	0.53	4.77	18.95	33.25	10.11	5.26
LY 2A	ab	48.35	2.00	13.46	12.35		0.17	9.30	9.80	3.02	1.06	0.48	4.83	20.03	30.24	10.59	4.84
gh24	mug	57.20	1.48	18.56	6.38		0.11	2.29	4.25	3.77	5.56	0.41	5.72	14.76	37.70	55.64	4.06
24 REP	mug	57.26	1.47	18.56	6.31		0.11	2.28	4.24	3.78	5.58	0.41	5.73	14.67	37.81	55.76	4.06
L17	mug	57.13	1.36	18.31	5.89		0.13	2.04	5.46	3.57	5.74	0.36	5.71	13.56	35.73	57.40	3.65
L16	ben	59.18	0.67	20.12	3.52		0.13	0.63	4.02	5.87	5.69	0.15	5.92	6.73	58.72	56.92	1.48
L63	ben	59.47	0.72	20.18	3.63		0.15	0.53	3.58	6.09	5.52	0.15	5.95	7.16	60.89	55.20	1.50
L3	tr	60.88	0.32	19.83	2.82		0.15	0.68	1.86	7.55	5.85	0.05	6.09	3.23	75.47	58.48	0.51
gh9	tr	61.09	0.34	20.01	2.93		0.15	0.48	1.38	7.72	5.84	0.05	6.11	3.35	77.18	58.43	0.51
L36	tr	60.58	0.35	19.73	4.02		0.12	0.33	2.11	6.83	5.87	0.06	6.06	3.48	68.32	58.66	0.62
gh20	tr	60.66	0.40	20.07	2.94		0.16	0.33	1.59	7.80	5.98	0.06	6.07	4.00	78.03	59.82	0.62
L39	pho	60.23	0.36	19.86	3.11		0.16	0.27	1.45	8.90	5.60	0.06	6.02	3.58	89.00	56.02	0.61
L18	pho	59.93	0.27	20.33	2.81		0.17	0.26	1.48	8.72	5.99	0.04	5.99	2.71	87.22	59.92	0.41
L38	pho	59.29	0.26	19.99	4.43		0.17	0.21	1.83	7.76	6.02	0.04	5.93	2.61	77.57	60.18	0.41
L38 REP	pho	59.54	0.26	20.15	3.98		0.18	0.21	1.85	7.82	5.96	0.05	5.95	2.65	78.22	59.62	0.52
L2	pho	58.45	0.28	20.60	3.34		0.14	0.20	2.08	9.05	5.82	0.04	5.85	2.79	90.47	58.25	0.41
L34	pho	59.26	0.30	20.86	2.86		0.15	0.18	1.42	8.89	6.03	0.04	5.93	3.01	88.94	60.34	0.42
L20	pho	59.18	0.29	20.76	3.26		0.15	0.16	1.33	8.73	6.09	0.04	5.92	2.94	87.28	60.92	0.41
gh23	pho	59.23	0.30	20.96	2.76		0.15	0.15	1.14	9.27	6.01	0.04	5.92	2.95	92.69	60.12	0.41
L31	pho	59.88	0.24	20.21	3.44		0.18	0.11	0.80	9.51	5.59	0.05	5.99	2.37	95.13	55.86	0.51
L55	tr	62.76	0.23	19.73	3.51		0.12	0.31	1.18	6.46	5.66	0.03	6.28	2.27	64.62	56.65	0.31
gh16	tr	63.48	0.30	18.84	2.94		0.21	0.18	1.04	7.29	5.68	0.04	6.35	2.96	72.91	56.77	0.41
L48	pho	61.69	0.26	19.42	3.27		0.22	0.17	1.18	8.15	5.58	0.05	6.17	2.60	81.55	55.76	0.51
L21	pho	59.96	0.29	19.77	3.28		0.30	0.15	1.02	9.81	5.40	0.03	6.00	2.87	98.11	53.98	0.31
gh21	tr	62.46	0.30	18.99	3.04		0.21	0.15	1.25	7.80	5.77	0.03	6.25	3.02	78.01	57.69	0.30
L33	pho	61.73	0.27	18.84	3.60		0.22	0.12	1.10	8.58	5.51	0.03	6.17	2.73	85.80	55.10	0.30
gh8	pho	61.55	0.27	19.39	3.30		0.25	0.09	1.11	8.39	5.62	0.03	6.16	2.66	83.94	56.23	0.31
L32	pho	59.82	0.19	19.96	3.41		0.26	0.06	1.12	9.85	5.29	0.05	5.98	1.86	98.50	52.87	0.51
gh7	pho	59.33	0.18	20.19	3.76		0.26	0.05	0.99	9.80	5.42	0.01	5.93	1.85	97.96	54.24	0.10
gh10	pho	59.76	0.19	20.28	3.35		0.25	0.05	0.89	9.87	5.34	0.02	5.98	1.86	98.68	53.36	0.21
L5	pho	59.39	0.18	19.94	4.08		0.25	0.04	1.42	9.53	5.16	0.01	5.94	1.80	95.32	51.57	0.10
gh11	pho	59.80	0.20	19.88	3.81		0.29	0.04	1.10	9.61	5.24	0.02	5.98	2.01	96.07	52.42	0.20

Figure 1. View of portion of Input data worksheet.

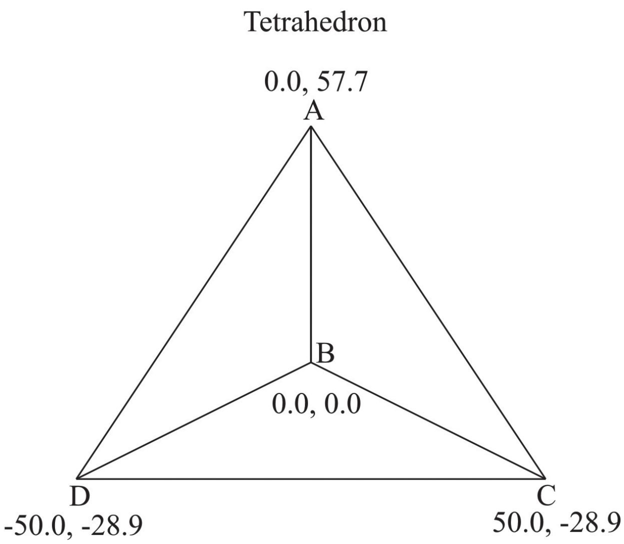

Figure 2. Tetrahedral diagram with coordinates.

normalized data for a triangle face (example BCD) of a tetrahedron are:

Y=(B×(28.8675)/((B+C+D)-28.8675)

X=(B×0+C×50+D×(-50))/(B+C+D)

Z=B×(-81.6497)/(B+C+D)

The equations for the transformation of unnormalized data to normalized data are provided in the Calculated data worksheet.

Then, the data are converted into X-Y coordinates using the following equations:

Y'=X×(cos(γ×π/180))×(-sen(β×π/180))×(-sen(α×π/180)) +sen(γ×π/180)×cos(α×π/180))+Y×(-sen(γ×π/180) ×(-sen(β×π/180))×(-sen(α×π/180))+cos(γ×π/180) ×cos(α×π/180))+Z×(cos(β×π/180)×(-sen(α×π/180)

X'=X×(cos(β×π/180)×cos(γ×π/180))+Y×(-sen(γ×π/180) ×cos(β×π/180))+Z×(sen(β×π/180))

where α, β, and γ are the angles for the rotation (Tetrahedron worksheets; column B, rows 3, 4, 5).

DROP DOWN MENU			UNNORMALIZED VALUES						NORMALIZED VALUES						CALCULATED COORDINATES			
READ ME			A	B	C	D	A+B+C+D	B+C+D	READ ME			READ ME			READ ME		READ ME	
	Sample name	Rock type	MgO	CaO	K2O	Na2O	tot	tot	Y	X	Z	Y	X	Z	X	Y	X	Y
SiO_2	L41	bsn	13.29	11.78	1.06	3.23	29	16	22	-4	-33	-8	-7	-60	-22	31	6	52
TiO_2	gh15	tph	8.45	10.78	1.34	1.73	22	14	18	-1	-39	-6	-1	-64	-18	38	6	58
Al_2O_3	gh14	bsn	7.47	13.62	1.13	2.26	24	17	14	-2	-45	-6	-3	-65	-14	42	5	59
Fe_2O_3	L37	tph	5.29	14.77	2.34	3.00	25	20	6	-1	-47	-8	-2	-60	-6	44	7	54
FeO	LY 2B	ab	11.25	9.59	1.01	3.33	25	14	21	-5	-31	-9	-8	-56	-21	29	7	48
MnO	LY 2A	ab	9.30	9.80	1.06	3.02	23	14	18	-4	-35	-8	-7	-58	-19	32	7	50
MgO	gh24	mug	2.29	4.25	5.56	3.77	16	14	-9	6	-22	-20	7	-26	10	22	21	25
CaO	24 REP	mug	2.28	4.24	5.58	3.78	16	14	-9	6	-22	-20	7	-25	10	22	21	24
Na_2O	L17	mug	2.04	5.46	5.74	3.57	17	15	-9	6	-27	-18	7	-30	10	26	19	29
K_2O	L16	ben	0.63	4.02	5.69	5.87	16	16	-18	-1	-20	-21	-1	-21	18	17	21	18
P_2O_5	L63	ben	0.53	3.58	5.52	6.09	16	15	-19	-2	-19	-22	-2	-19	19	15	21	15
SiO2/10	L3	tr	0.68	1.86	5.85	7.55	16	15	-22	-5	-10	-25	-6	-10	20	5	24	5
TiO2*10	gh9	tr	0.48	1.38	5.84	7.72	15	15	-24	-6	-7	-26	-6	-8	22	3	24	3
Na2O*10	L36	tr	0.33	2.11	5.87	6.83	15	15	-23	-3	-11	-25	-3	-12	22	8	24	8
K2O*10	gh20	tr	0.33	1.59	5.98	7.80	16	15	-24	-6	-8	-26	-6	-8	22	4	24	4
P2O5*10	L39	pho	0.27	1.45	5.60	8.90	16	16	-25	-10	-7	-26	-10	-7	22	1	24	1
	L18	pho	0.26	1.48	5.99	8.72	16	16	-25	-8	-7	-26	-8	-7	23	2	24	2
READ ME	L38	pho	0.21	1.83	6.02	7.76	16	16	-24	-5	-9	-25	-6	-10	23	5	24	5
	L38 REP	pho	0.21	1.85	5.96	7.82	16	16	-24	-6	-10	-25	-6	-10	23	5	24	5
	L2	pho	0.20	2.08	5.82	9.05	17	17	-24	-9	-10	-25	-10	-10	22	4	23	4
	L34	pho	0.18	1.42	6.03	8.89	17	16	-25	-9	-7	-26	-9	-7	23	1	24	1
	L20	pho	0.16	1.33	6.09	8.73	16	16	-26	-8	-7	-26	-8	-7	23	1	24	1
	gh23	pho	0.15	1.14	6.01	9.27	17	16	-26	-10	-6	-27	-10	-6	23	0	24	0
	L31	pho	0.11	0.80	5.59	9.51	16	16	-27	-12	-4	-27	-12	-4	24	-3	24	-3
	L55	tr	0.31	1.18	5.66	6.46	14	13	-24	-3	-7	-26	-3	-7	23	4	25	4
	gh16	tr	0.18	1.04	5.68	7.29	14	14	-26	-6	-6	-27	-6	-6	24	1	25	1
	L48	pho	0.17	1.18	5.58	8.15	15	15	-26	-9	-6	-27	-9	-6	23	1	24	1
	L21	pho	0.15	1.02	5.40	9.81	16	16	-26	-13	-5	-27	-14	-5	23	-2	24	-2
	gh21	tr	0.15	1.25	5.77	7.80	15	15	-26	-7	-7	-26	-7	-7	24	2	24	2
	L33	pho	0.12	1.10	5.51	8.58	15	15	-26	-10	-6	-27	-10	-6	23	0	24	0
	gh8	pho	0.09	1.11	5.62	8.39	15	15	-26	-9	-6	-27	-9	-6	24	0	24	0
	L32	pho	0.06	1.12	5.29	9.85	16	16	-27	-14	-6	-27	-14	-6	23	-2	23	-2
	gh7	pho	0.05	0.99	5.42	9.80	16	16	-27	-13	-5	-27	-13	-5	23	-2	24	-2
	gh10	pho	0.05	0.89	5.34	9.87	16	16	-27	-14	-4	-27	-14	-5	23	-3	24	-3
	L5	pho	0.04	1.42	5.16	9.53	16	16	-26	-14	-7	-26	-14	-7	23	0	23	0
	gh11	pho	0.04	1.10	5.24	9.61	16	16	-27	-14	-6	-27	-14	-6	23	-2	23	-2

Figure 3. View of portion of Calculated data worksheet.

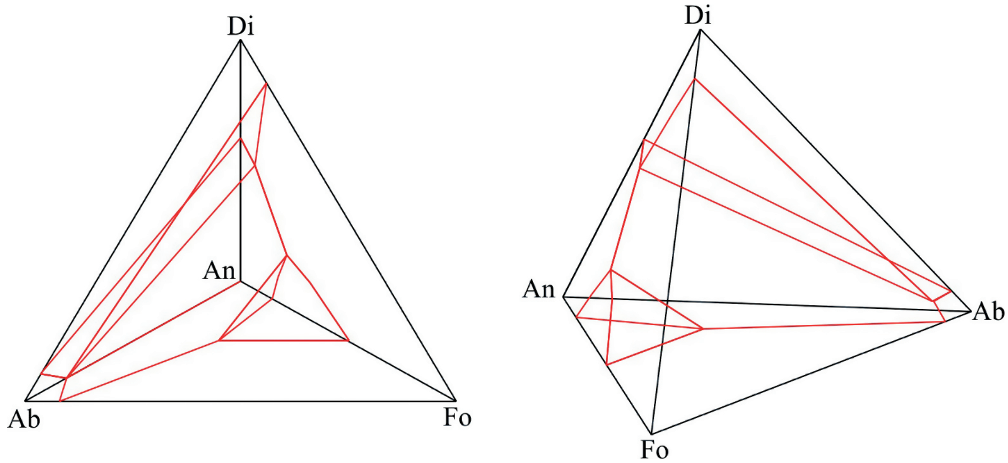

Figure 4. Di-Ab-Fo-Ab system drawn with Tetra-Plot before and after rotation.

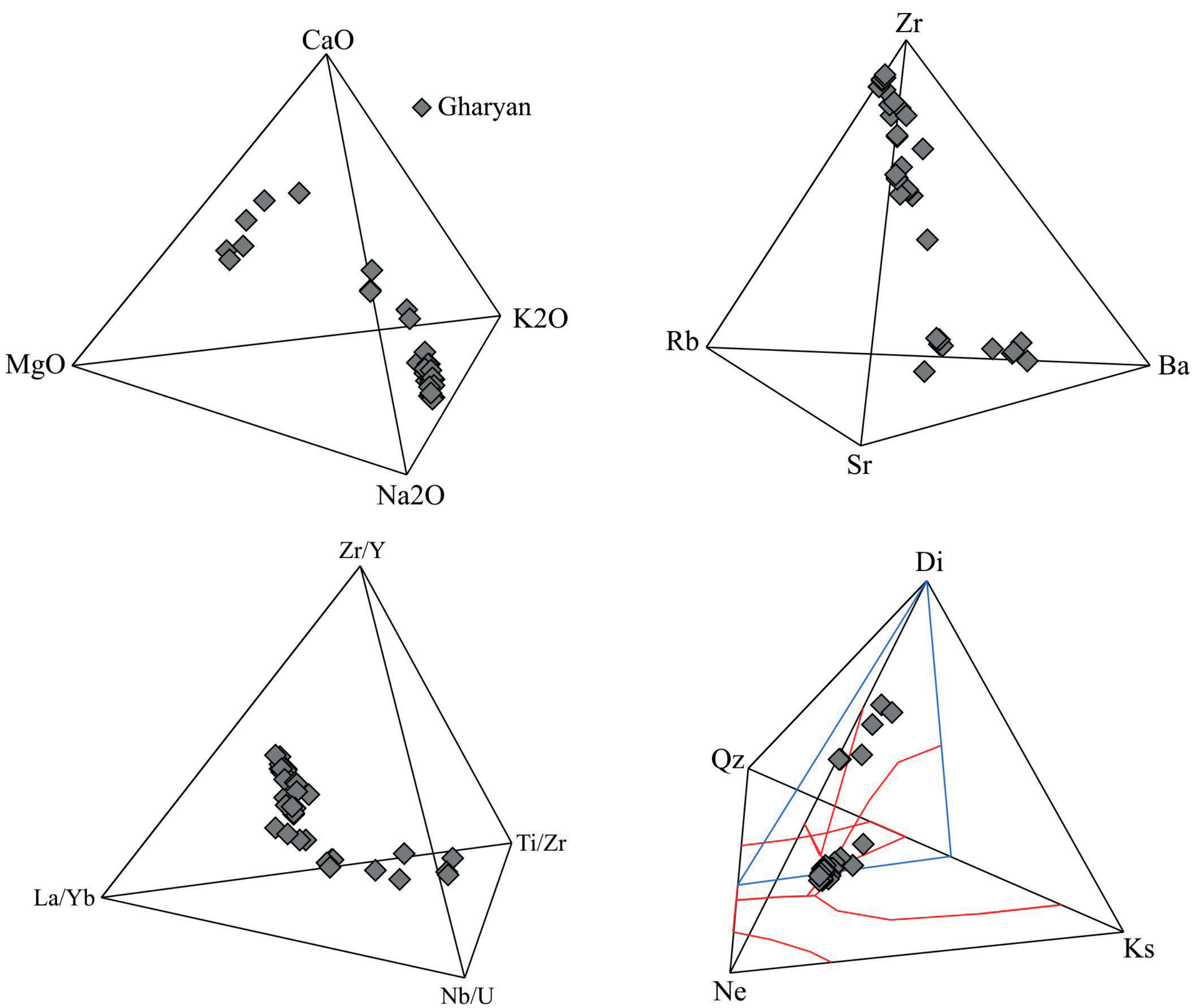

Figure 5. Examples of tetrahedral diagrams for the igneous rocks from the Gharyan volcanic field. Data are from Lustrino et al. (2012).

Rotation of the tetrahedron

The elementary 3D rotation matrix is constructed to perform rotations individually about the three coordinate axes. The tetrahedron can rotate changing the angle values in the column B, rows 3-5 of the Tetrahedron worksheet.

In Figure 4 is shown the system Di-An-Fo-Ab before and after rotation of angles α (8°), β (143°) and γ (338°).

The user can design lines (e.g. cotectics), points (e.g., eutectics, peritectics) in a phase system by inserting the required plotting coordinates in the Input data worksheet. In the Tetrahedron CIPW worksheet, the coordinates required for the cotectic lines and eutectic points of Di-Qz-Ne-Ks and Di-Fo-An-Ab systems are reported in the Note worksheet.

IMPLICATIONS

Tetra-Plot spreadsheet provides a practical and simple method to plot tetrahedral diagrams. This program increases the ability of the user to easily display and interpret data for complex systems. Tetrahedral diagrams are useful for mineralogists, geochemists and petrologists to classify mineral or rock types and to investigate igneous and/or metamorphic processes.

Examples of tetrahedral diagrams generated by Tetra-Plot showing data of volcanic rocks from the Gharyan volcanic field (Lustrino et al., 2012) are represented in Figure 5.

ACKNOWLEDGMENTS

The author is grateful to Michele Lustrino, which helped to improve the early versions of this paper and program, as well as Leone Melluso for his helpful comments and suggestions. An anonymous reviewer and the Section Editor Silvio Mollo provided valuable critical review. This work was granted by Fondi Ricerca Dipartimentale 2015.

REFERENCES

Armienti P. (1986). TETRASEZ an interactive program in BASIC to perform tetrahedral diagrams. Computer & Geosciences 12, 229-241.

France L., Ouillon N., Chazot G., Kornprobst J. and Boivin P. (2009). CMAS 3D, a new program to visualize and project major elements compositions in the CMAS system. Computers & Geosciences 35, 1304-1310.

France L. and Nicollet C. (2010). MetaRep, an extended CMAS 3D program to visualize mafic (CMAS, ACF-S, ACF-N) and pelitic (AFM-K, AFM-S, AKF-S) projections. Computers & Geosciences 36, 786-791.

Lustrino M., Cucciniello C., Melluso L., Tassinari C.C.G., dè Gennaro R. and Serracino M. (2012). Petrogenesis of Cenozoic volcanic rocks in the NW sector of the Gharyan volcanic field, Libya. Lithos 155, 218-235. doi:10.1016/j.lithos.2012.09.003

Shimura T. and Kemp A.I.S. (2015). Tetrahedral plot diagram: A geometrical solution for quaternary systems. American Mineralogist 100, 2545-2547.

Torres-Roldan R.L., Garcia-Casco A. and Garcia-Sanchez P.A. (2000). CSpace: an integrated workplace for the graphical and algebraic analysis of phase assemblages on 32-bit wintel platforms. Computers & Geosciences 26, 779-793.