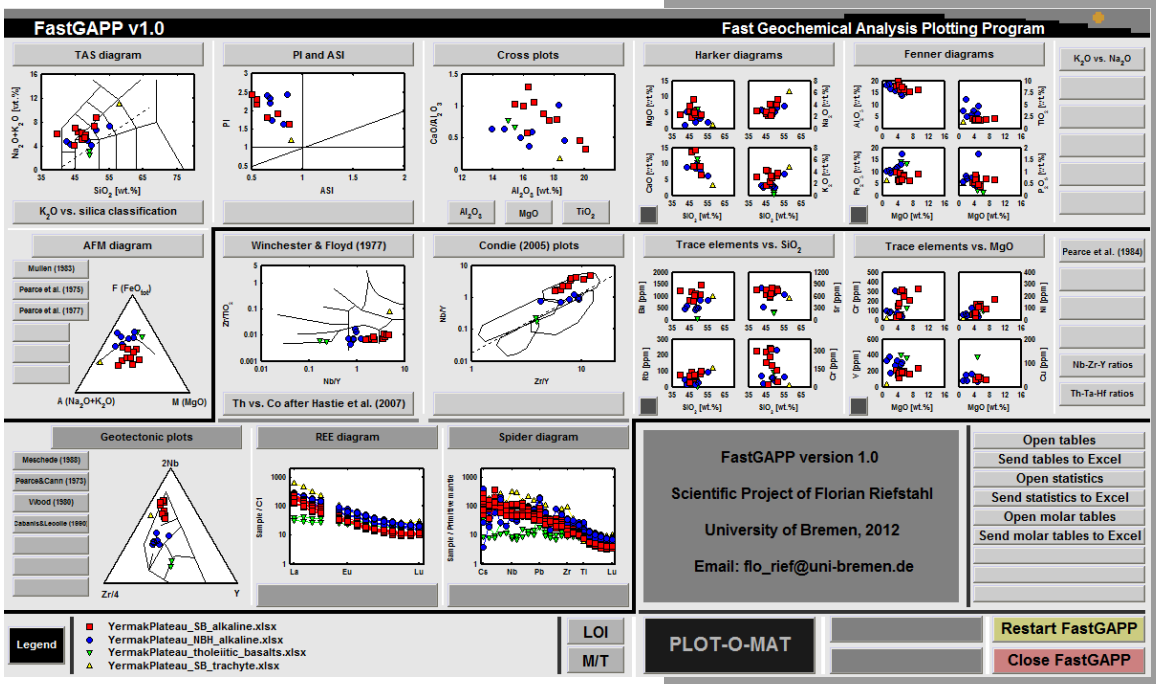
Universität Bremen

FastGAPP

A user-friendly MATLAB-based program helps geo scientists classifying, interpreting and displaying igneous rocks in terms of petrography and geochemistry



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Cover image: Main window of FastGAPP with geochemical data of alkaline basalts, two tholeiitic basalts, and one trachyte from the Yermak Plateau (Riefstahl et al., submitted). The fields and lines are digitized from several publications (Condie, 2005; Fitton et al., 1997; Irvine and Baragar, 1971; Le Bas et al., 1986; MacDonald, 1968; Meschede, 1986; Pearce et al., 1977). Chondrite and primitive mantle normalization values in rare earth element diagram and spider diagram are taken from Sun & McDonough (1989). The peralkalinity index (PI) and the alumina saturation index (ASI) are calculated after Shand (1927; 1943).

“The whole is greater than the sum of its parts.”

- Aristotle

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Summary

Specific programs for the evaluation of geochemical data of igneous rocks are rare, some are difficult to use, and the licenses are very expensive. Additionally, changing advanced settings of the created plots and the comparison with publicized data are extremely time-intensive and therefore, also expensive.

FastGAPP (Fast Geochemical Analysis Plotting Program), a MATLAB-based program has been written during this geoscientific project. FastGAPP automatically reads geochemical datasets from sorted Excel Spreadsheets, normalizes the data volatile-free, and plots up to 4 datasets in the common geochemical and geotectonic classification diagrams. Fields in predefined diagrams are digitized from several publications and integrated in FastGAPP. With the PLOT-O-MAT function it is possible to plot elements or elemental ratios into linear, semi logarithmic, logarithmic and ternary diagrams, interactively. Another integrated program Petro Plot allows displaying petrographic observations from volcanic, plutonic, gabbroic, or ultramafic rocks. Therefore, the first Version of FastGAPP yields an interesting, very user-friendly base with many applications in research and teaching of whole-rock geochemistry and petrography.

With the existing MATLAB scripts it is easily possible to extent the diversity of plots integrated in future versions FastGAPP to gain new applications. Latter extensions might include more classification plots (e.g., for metamorphic rocks, for specific minerals like amphiboles, pyroxenes, or garnets), model runs for main elements and trace elements, plotting of isotope data (e.g., Rb-Sr, Sm-Nd, K-Ar, Ar-Ar) and much more.

1. System requirements

1.1 Requirements for FastGAPP

Software requirements:

- Mathworks MATLAB (R2011a or latter release)
- Any Microsoft Excel (supporting .xls- or .xlsx-format)

Hardware requirements:

- Minimum hardware requirements are given by the combined requirements of Mathworks MATLAB (see 1.2) and Microsoft Office (see 1.3)

Recommended requirements:

- Any Intel or AMD multi-core processor (better than 2 GHz) supporting 64-bit
- 4 GB RAM (or more)
- 8 GB RAM disk space (for full installation of Microsoft Office and MATLAB)
- 1440 x 900 or higher resolution monitor
- 64-bit operating system
- 64-bit version of Microsoft Office and MATLAB

1.2 Requirements for MATLAB (R2012a)

http://www.mathworks.de/products/matlab/requirements.html

General requirements:

- Window XP, Windows 7 (32-bit or 64-bit)
- Any Intel or AMD x86 processor supporting “Streaming SIMD Extensions 2” (SSE2)
- 1 GB disk space (for MATLAB only)
- 1024 MB RAM (2048 MB RAM recommended)

1.3 Requirements for Microsoft Office 2010

http://technet.microsoft.com/en-us/library/ee624351.aspx

General requirements:

- Windows XP, Windows 7 (32-bit or 64-bit)
- Any 500 MHz processor or better
- 3,5 GB disk space (for Microsoft Office Professional Plus 2010)

2. Introduction

2.1 Why is FastGAPP useful?

Geochemical studies of igneous rocks are fundamental to classify rock types in terms of main-, minor-, trace element whole-rock chemistry. Together with petrographic observations from thin sections it is possible to classify igneous rocks and to draw interpretations about:

- **The petrogenesis and evolution of igneous rocks.**
- **The thermal and barometric conditions in which a primary magma have formed.**
- **The magmatic processes that might be involved in the evolution of igneous rocks.**
- **The geotectonic environment in which igneous rocks might have formed.**

Analytical methods, therefore, were enhanced and improved during the last centuries. However, x-ray fluorescence (XRF) and inductively coupled plasma–mass spectrometry (ICP-MS) might be the most prominent and effective methods to explore the chemistry of whole-rock samples. But the evaluation and a comparison with other geochemical data of similar igneous rocks need a lot of time because most available software (e.g., Microsoft Excel or Golden Software Grapher) are developed for broad applications and not for specific geochemical analyses. Changing settings of plots is also time-consuming and, therefore, very expensive. Nevertheless, specific plots (fields and/or lines) have to be digitized first. And then, they also have to be plotted into diagrams which might need also a lot of time.

A solution for these time-consuming problems is the **Fast Geochemical Analysis Plotting Program** (FastGAPP) which uses MATLAB as a machine-independent platform. The fast processing and displaying of data which FastGAPP performs is an interesting alternative to conventional programs. The time required for geochemical analyses and comparison with published data will be shortened significantly. The geochemical data only have to be sorted in a simple input norm (an Excel Spreadsheet) and then, FastGAPP will read the input and plot it in many varieties. Digitized datasets from about twenty publications are stored in the scripts and can, therefore, be plotted together with the data.

2.2 What is MATLAB?

MATLAB is the abbreviation for "***Mat****rix* ***Lab****oratory*", a commercial fourth-generation programming language developed by Mathworks. It is a command line based programming language for numerical computing, calculation and manipulation of matrices, plotting of data and functions, implementation of algorithms and programming of graphical user interfaces (GUI). The simplified mathematically oriented syntax enables plainer writing of complex programs than in other programming languages. Commands can be saved as scripts or functions, and therefore, MATLAB supports batch programming. MATLAB can also interface with other programming languages like C, C++, Java and FORTRAN. Thus, MATLAB has broad fields of application in all disciplines of science, engineering and economy.

There is an example (Fig. 1) below that describes the main window, the modules and the functionality of MATLAB. However, MATLAB is a powerful very complex program which will not be explained in detail in this manual. But the example simply explains how FastGAPP works. FastGAPP reads data from an Excel worksheet and split the columns into different variables and plot the data into many predefined diagrams.

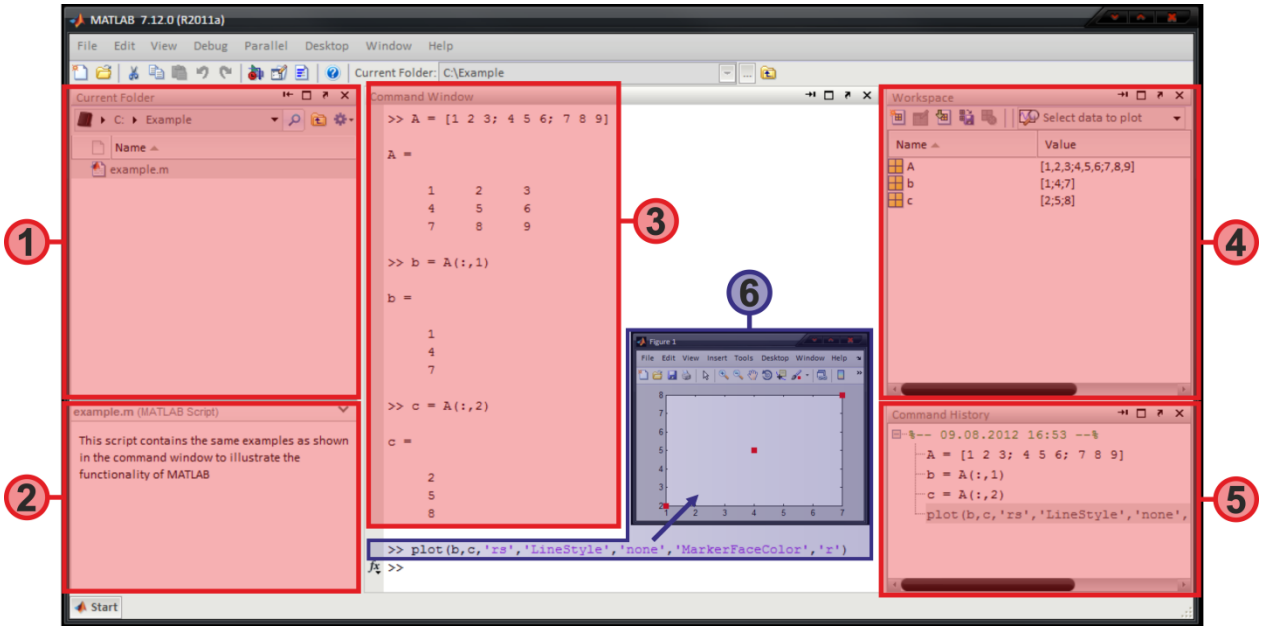

Fig. 1: An example to explain the main window of MATLAB. The current folder (1) and the documentation of a MATLAB function (2) are shown on the left side of the main window. The command window (3) in the middle is needed to test any commands without saving them into any function. In this example a 3x3 matrix A is created, and then, the first and second column are extracted from it. These three variables are stored in the MATLAB workspace (4). The command history (5) records commands that have previously been used. With the last command (*"plot"*) a new MATLAB figure (6) is opened that with the created variable b on the x-axis and variable c on the y-axis. This is a very simplified example but it illustrates how FastGAPP works in general.

3. Functionality of FastGAPP

First of all, FastGAPP reads data from the different columns of the input form (an Excel Spreadsheet). Second, the raw data are normalized volatile-free to hundred weight per cent, main elements are converted to molar per cent, input and output statistics are created, and, finally, reassembled to tables. During these processes all geochemical data (raw data, normalized data, molar data, statistics and tables) are saved as independent variables in the workspace of MATLAB. During the opening process of the FastGAPP main window variables are read from the MATLAB workspace (and if needed, calculated) and displayed in different plots for a first overview of the geochemical data. After the main window has been finally opened, it is possible to open and display several classification and variation diagrams by a click on any of the buttons. These diagrams are opened in separate MATLAB figures. The process structure of FastGAPP and a detailed step-by-step explanation how to use FastGAPP are shown in the following subchapters.

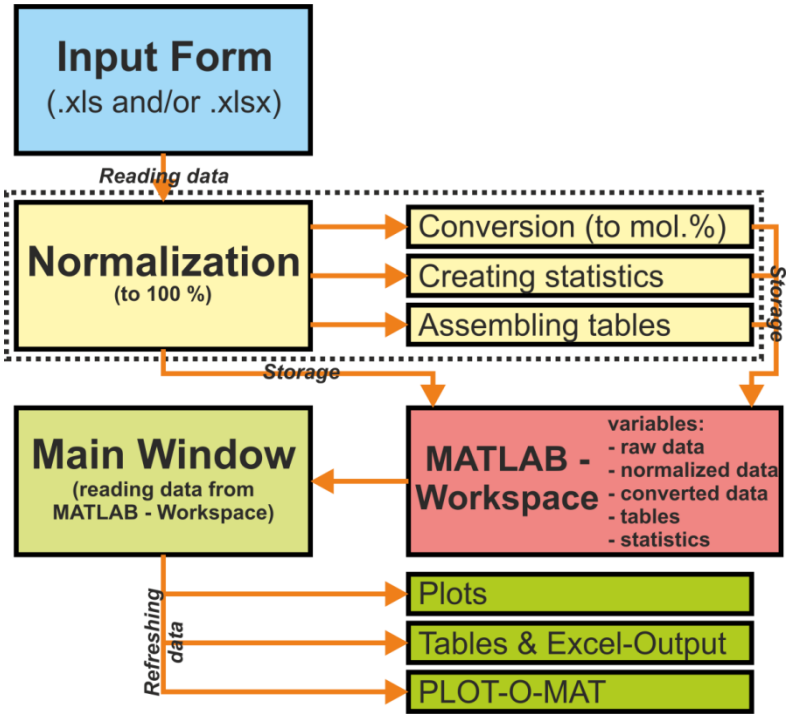

Fig. 2: Schematic illustration of the process structure of FastGAPP.

3.1 Sort sequence of the FastGAPP input form

The preparation of a dataset is the most time-consuming but also the most important step for using FastGAPP. It has to be performed manually with highest attention, concentration, and reliability. However, there are many different solutions to prepare an input for FastGAPP. In chapter 3.2 there is one of the possibilities explained in detail.

The input form of FastGAPP contains 82 columns, six columns (Excel columns A–F) for non-numerical data (e.g. for sample labels, location, laboratories or other information) and 76 columns (Excel columns G–CD) for numerical data (geochemical data). The whole sort sequence is visualized in Fig. 3 and Appendix 1. Note that any numerical data in any of the first six columns will result in an error during the continuing process! The geochemical data has to be sorted as follows:

- **Column G–P:** Main element oxides in most common sort sequence (in wt. %)
- **Column Q–V:** Volatiles (in wt. %)
- **Column W:** Total values (in wt. %)
- **Column X–BJ:** Trace elements sorted alphabetically (in ppm)
- **Column BK–BP:** Platinum group elements sorted by increasing atomic number (ppm)
- **Column BQ-CD:** Rare earth elements sorted by increasing atomic number (ppm)

Note that main element oxides, volatiles and the total value are given in weight per cent while all trace elements are given in parts per million (mg/kg). Also recognize that the input form requires total iron as Fe_2O_3 (often given as FeO), sulfur as SO_3 and chromium as Cr (often given as Cr_2O_5). If the data differ, a recalculation using stoichiometric factors for each element or oxide is needed.

Attention: In cell CE2, a green zero is stored. This green zero extends the variable that is latter created by FastGAPP to the Excel column CE and will be removed during the normalization of the data. Do not clear it!

3.2 Preparation of the FastGAPP input

The input forms for FastGAPP are stored in the folder *C:\FGAPP\input_forms* as write-protected xls- and xlsx-files. For the preparation of a dataset for FastGAPP open the preferred file format, and save it using a different file name into any folder on the computer or into the predefined folder (*C:\FGAPP\geochemical_data*).

In the next step, open the created file and copy the new data with header lines and paste it into the input form (line #2). Sort the data as explained in chapter 3.1 and visualized in Fig. 3. Take care that the FastGAPP header line of the input form is not changed during the preparation but copy and insert the old header lines to avoid any confusion. When the preparation is finished, make sure that every element and oxide is in the correct column with the correct unit. Do not mind about blank cells, rows, columns, and/ or non-numerical values (e.g. <5, ND or DL) where some values might not be determined or are below the detection limit. These cells are turned into not-a-number (NaN) during the normalization process. Finally, confirm that the data is correct, clear old header lines (Fig. 4) and save the file again. Then the input form is finally prepared for FastGAPP.

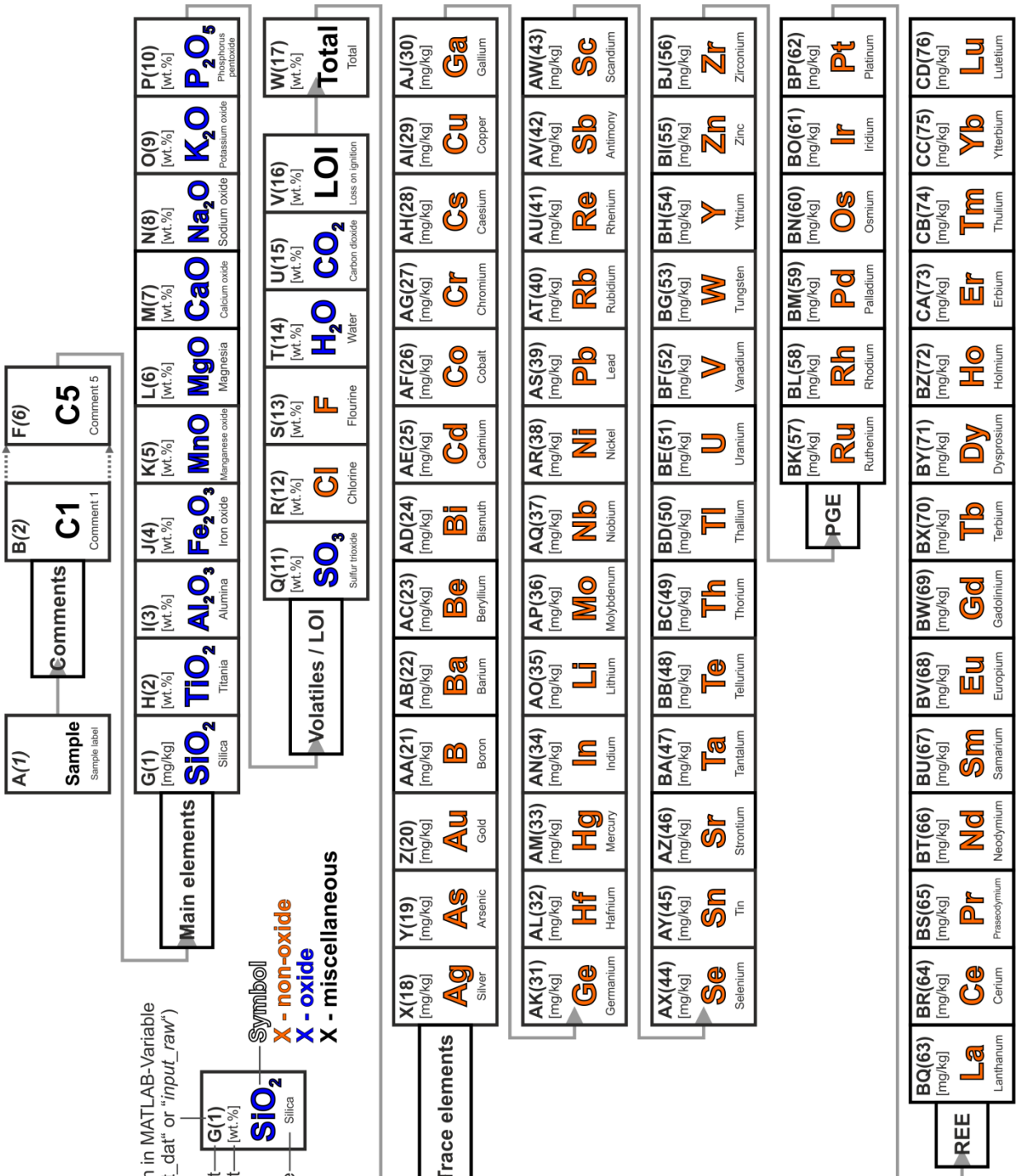

Fig. 3: Sort sequence of the FastGAPP input form. Abbreviations: PGE = platinum group elements; REE = rare earth elements.

A

	G	H	I	J	K	L	M	N	O	P
1	SiO_2 [wt.%]	TiO_2 [wt.%]	Al_2O_3 [wt.%]	Fe_2O_3 [wt.%]	MnO [wt.%]	MgO [wt.%]	CaO [wt.%]	Na_2O [wt.%]	K_2O [wt.%]	P_2O_5 [wt.%]
2	SiO2	TiO2	Al2O3	Fe2O3	MnO	MgO	CaO	Na2O	K2O	P2O5
3	%	%	%	%	%	%	%	%	%	%
4	48.58	2.05	15.27	14.05	0.19	4.82	10.26	2.53	0.50	0.21
5	48.44	1.70	14.82	13.12	0.19	6.20	11.36	2.24	0.27	0.15

B

	G	H	I	J	K	L	M	N	O	P
1	SiO_2 [wt.%]	TiO_2 [wt.%]	Al_2O_3 [wt.%]	Fe_2O_3 [wt.%]	MnO [wt.%]	MgO [wt.%]	CaO [wt.%]	Na_2O [wt.%]	K_2O [wt.%]	P_2O_5 [wt.%]
2	48.58	2.05	15.27	14.05	0.19	4.82	10.26	2.53	0.50	0.21
3	48.44	1.70	14.82	13.12	0.19	6.20	11.36	2.24	0.27	0.15
4										
5										

Fig. 4: Example for a correctly prepared input form. The main elemental data in example A is well sorted but the old header records are still in Excel line #2 and #3. It is required to clear the two rows. Example B shows the final sheet after having cleared the old header. The geochemical dataset is now prepared for FastGAPP and can be used after having saved the file.

3.3 Opening of FastGAPP

First, start MATLAB and wait until it is initialized. After that, change the current folder to *C:\FGAPP* (Fig. 5) in MATLAB. When the current folder is changed, type *fgapp* into the MATLAB command window and press *enter* to run the script *C:\FGAPP\fgapp.m* (Fig. 5). After having pressed *enter*, the FastGAPP initialization window opens for choosing how many datasets should be processed on the left side (Fig. 6). Alternatively, the start button for Petro Plot is placed on the right side (see chapter 4). Prior to a comparison of more datasets, it is recommended using FastGAPP with a single dataset to get familiar with the program. Therefore, the functionality for a single dataset with only two samples is explained in the next examples. By a click on the “1 dataset” button (Fig. 6) a standard dialog window for the selection of a file opens (Fig. 7). According to the number of datasets more file selection windows will open in succession. Navigate through the folders to choose the file and click on open. Note that the selection window will always open in *C:\FGAPP*. Thus, saving of the prepared files into the predefined folder will be easier to handle. After a file has been chosen, the initialization process of FastGAPP starts and results in an output (to the MATLAB command window) of the current time and the elapsed time that has been needed for reading, calculating and opening of the main window.

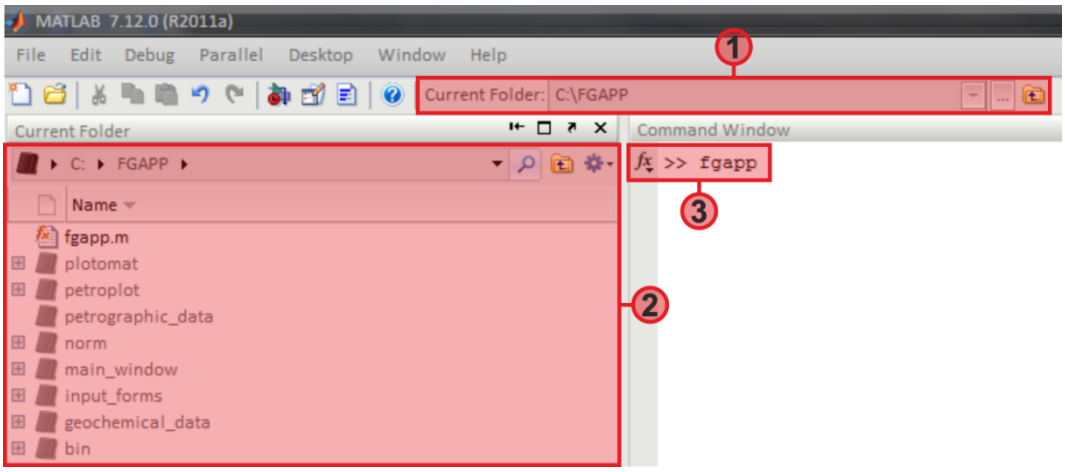

Fig. 5: Screenshot of the MATLAB main window. The current folder can be changed in the MATLAB control elements and menus (1 or 2). After having chosen the current folder, it is displayed with all contained subfolders in the current folder menu (2). To start FastGAPP, change the current folder to the location on the system where FastGAPP is saved, then type *fgapp* in the command window (3) and press *enter* to run FastGAPP. In the next step the initialization window will open (Fig. 6).

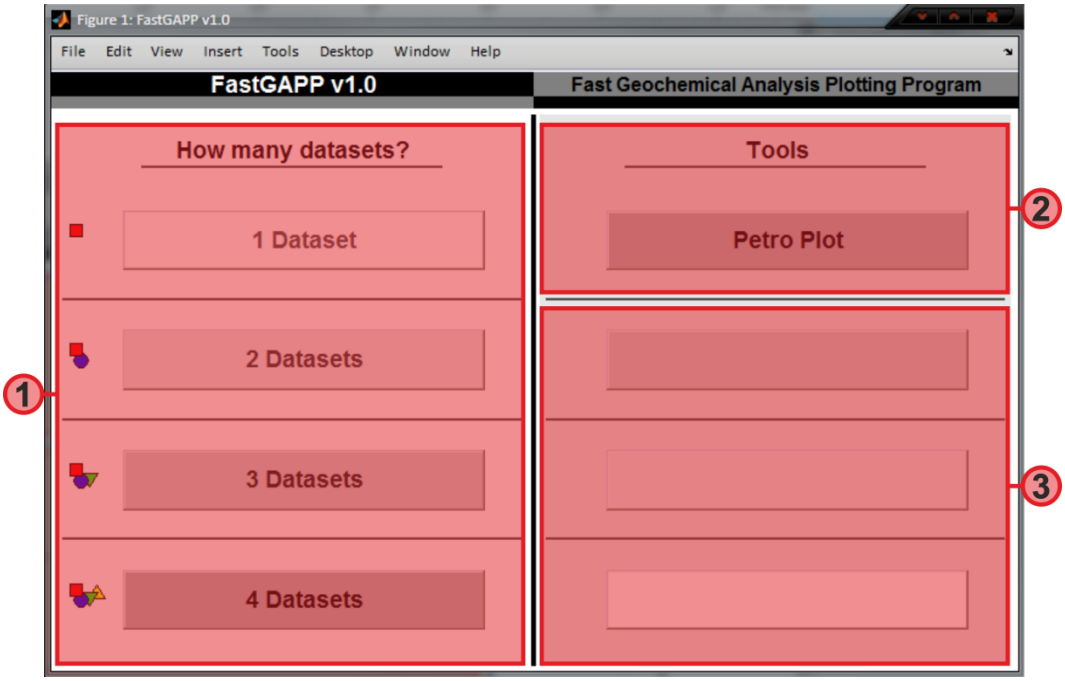

Fig. 6: Initialization window of FastGAPP. On the left side (1) it is possible to choose how many dataset should be opened with FastGAPP. With a click on any of these four buttons file selection window/ windows will open to choose files (Fig. 7). To start Petro Plot and display petrographic data (see chapter 4) press the uppermost button on the right side (2). The three blank buttons (3) are reserved for future versions of FastGAPP.

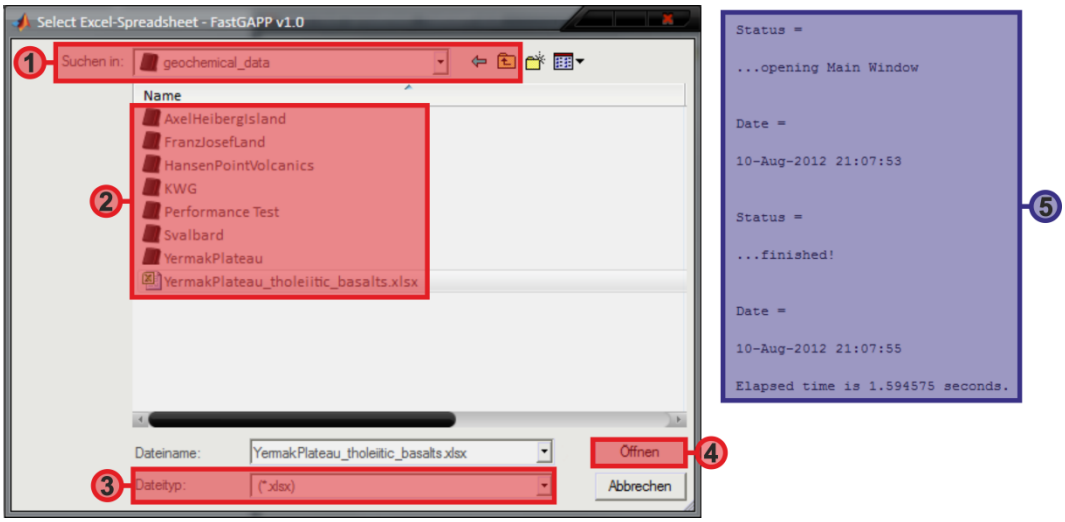

Fig. 7: Screenshots of the file selection window of FastGAPP and the final dialog after having selected a file. First navigate to the folders (1) where the geochemical data is saved and select a file with a click on it (2). Note that only xlsx-files are displayed until the file types are not changed (3). Second, click on open (4). A double-click on a file is also possible for opening. If more than one dataset is chosen, the file selection window will open several times to load more datasets. Subsequently, FastGAPP starts to read the data, performs the normalization of the data, and finally, opens the main window (Fig. 8). The process has been successful when finally the dialog (5) is displayed in the MATLAB command window. Note that this is a German language version of Windows 7 with a modified design. The language, labels and appearance differ from other operating systems.

3.4 Reading, normalization, and recalculation of the data

After the selection of a file (or up to 4 files), FastGAPP will read the file and, normalize and recalculate the contained data (Fig. 2), afterwards. During this process FastGAPP switches through several subfolders in *C:\FGAPP*. After reading, FastGAPP switches from the folder *C:\FGAPP\mainwindow* (where the initialization files for FastGAPP are stored) to the folder *C:\FGAPP\norm*. This folder contains the scripts which perform the normalization process, the conversion of the data, the compilation of data statistics, and finally, the re-assemblage to tables (Fig. 2).

The normalization scripts work slightly simple: The imported numerical data table (e.g. “input_dat1” for the first dataset) from the Excel file is splitted into 76 single column variables in MATLAB (e.g. “r1SiO2” is the raw silica content of the first file). Then the NaN entries are turned to zero for calculating the total percentage of main and trace elements (because any calculation with NaN values will result in NaN). FastGAPP performs a volatile-free normalization. Therefore, SO_3, Cl, F, H_2O, CO_2 and the loss on ignition (LOI) are ignored during calculation of the total percentage. Afterwards the raw data is normalized to 100 wt. % column by column (e.g. “n3Zr” is the normalized zirconium content of the third dataset) and, finally, reassembled to complete

tables (for later displaying of the normalized data in FastGAPP and/ or export exporting the data back to Excel file). During this process the main elements are also converted to molar per cent by dividing the values by their molar weights (the recommend values by the International Union of Pure and Applied Chemistry) and then normalizing these molar proportions to 100 molar per cent (e.g. “x4MnO” is molar percentage of manganese oxide of the fourth dataset). All created variables and used MATLAB commands are recorded in the glossary (chapter 6).

3.5 Opening and description of the main window

After the normalization process the initialization of the main window starts. During the initialization variables are read from the MATLAB workspace and will be plotted into several

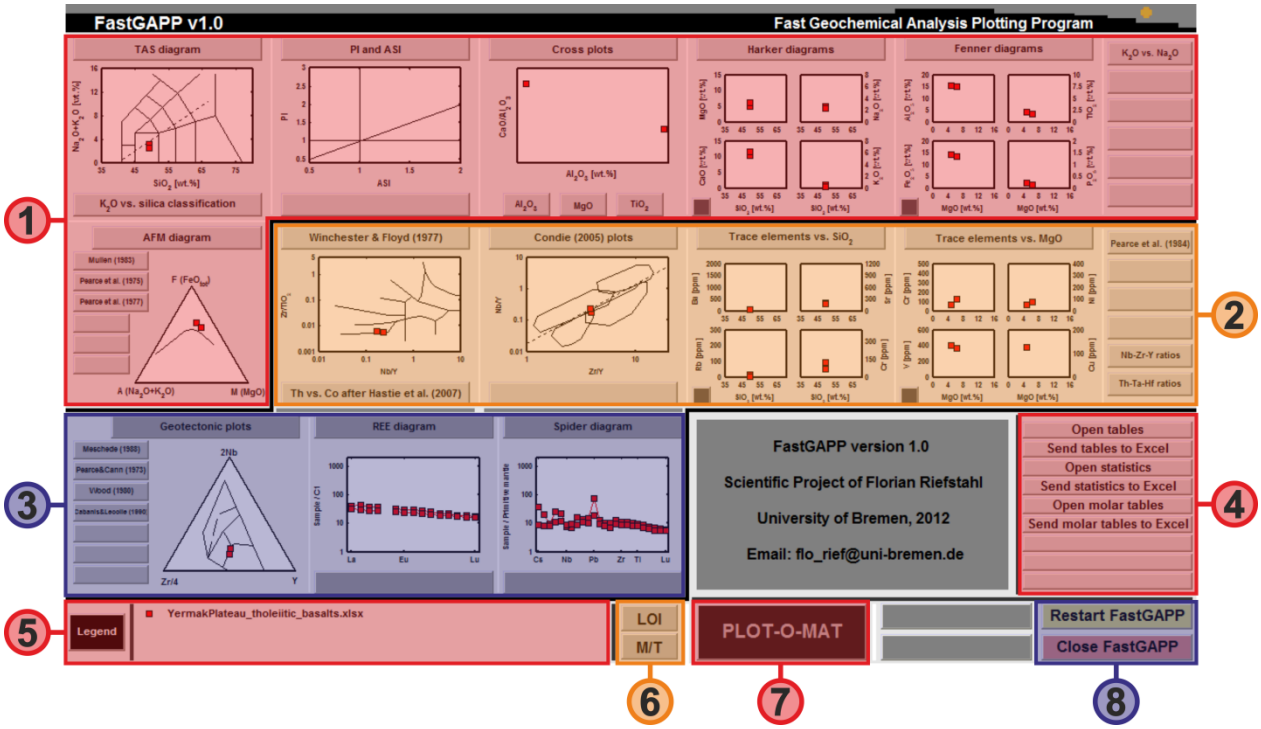

Fig. 8: Screenshot of the FastGAPP main window with an exemplary dataset including two tholeiitic basalts dredged from the Yermak Plateau (Riefstahl et al., submitted). In the uppermost part (1) several plots and buttons for main and minor elements are located. In contrast, in the middle part (2) and lower part (3) buttons for trace element classification, trace element variations and ratios, geotectonic classification, REE-diagrams and spider diagrams are placed. On the right side of the lower part (4) of the main window it is possible to open tables for raw, normalized, molar data and data statistics or to send the recalculated data back to Excel. In the lowermost part there are miscellaneous buttons for opening a separate figure of the legend (5), for discussions on the LOI and main and trace element distribution (6), for initializing the PLOT-O-MAT (7), and for restarting and closing of FastGAPP (8). The fields and lines are digitized from several publications (Condie, 2005; Fitton et al., 1997; Irvine and Baragar, 1971; Le Bas et al., 1986; MacDonald, 1968; Meschede, 1986; Pearce et al., 1977). Chondrite and primitive mantle normalization values are taken from Sun & McDonough (1989) and the peralkalinity index (PI) and the alumina saturation index (ASI) are after Shand (1927; 1943).

diagrams of the FastGAPP main window (Fig. 8) that will give an overview of the imported geochemical data. It is possible to find any mistakes that are made during the preparation of the dataset. Several of the most important classification diagrams are shown in the main window (Fig. 8). It is sorted thematically by distribution of elements. The uppermost diagrams and buttons are reserved for main and minor elements (e.g. total alkali versus silica diagram, Harker-diagrams, Fenner-diagrams). The middle part is reserved for trace elements (e.g. trace element classification, trace element variations over SiO_2 and MgO and ratios of the high field strength elements). In the lower part buttons and diagrams for geotectonic classification, REE pattern, and the spider-diagram are placed. On the right side of the lower part buttons for opening tables in FastGAPP and export to Excel buttons are located. In the lowermost part miscellaneous buttons are placed (legend of the datasets, discussions on LOI and distribution of main and trace elements, the opening button for the PLOT-O-MAT and the restart/ close buttons). Note that some data might be located outside of the diagrams in the main window because some axes are fixed for a better displaying of the data. Note that blank buttons are reserved for future versions of FastGAPP.

3.6 Plots contained in FastGAPP

When the main window is opened, FastGAPP switches to the folder *C:\FGAPP\bin* where the scripts for the predefined diagrams are stored. By pressing any of the labeled buttons of the FastGAPP main window one or more predefined plots or tables will open. Before a plot is opened in a new MATLAB figure, the data will be refreshed by running the normalization scripts again (see Fig. 2). This repeated normalization is integrated to avoid an accidental overwriting of the created variables and might take some time if large datasets are loaded. But for most datasets it runs very fast. When the repeated normalization is finished, the data for the different plots are calculated (e.g. $N_2O + K_2O$ for total alkalis versus silica diagram) or normalized (e.g. for ternary diagrams or for normalization to primitive mantle) and finally new MATLAB figures are opened which can be modified or exported into supported image or vector graphics format (see chapter 5).

FastGAPP contains over one hundred predefined linear, semi-logarithmic, logarithmic or ternary diagrams. Therefore, more than thousand data points of fields and lines are taken from about 20 publications and integrated into the program structure. All buttons and their associated plots are explained in Tab. 1 and for further explanations one example is shown in Fig. 9.

Tab. 1: All buttons of FastGAPP with a short description and references for the contained plots.

Button Name	Data	Description
TAS diagram	**N**	7 figures for classification of igneous rocks using total alkalis (Na_2O + K_2O) versus silica in several arrangements with the division line after MacDonald (1968), division line after Irvine & Baragar (1971), fields for volcanic rocks after Le Bas et al. (1986) and fields for volcanic and plutonic rocks after Middlemost (1994).
K_2O vs. silica classification	**N**	1 figure for classification of subduction related volcanic rocks using K_2O versus silica after Peccerillo & Taylor (1976).
PI and ASI	**M**	1 figure for classification of the molar character of igneous rocks to divide into peralkaline, metaluminous and peraluminous rocks using the peralkalinity index (PI) versus alumina saturation index (ASI) index after Shand (1927; 1943).
Cross plots	**N**	3 figures to display all main elements normalized to Al_2O_3, MgO, and TiO_2
Al_2O_3	**N**	Same as “Cross plots” but only 1 figure with main elements normalized to Al_2O_3.
MgO	**N**	Same as “Cross plots” but only 1 figure with main elements normalized to MgO.
TiO_2	**N**	Same as “Cross plots” but only 1 figure with main elements normalized to TiO_2.
Harker diagrams	**N**	1 figure with the Harker variation diagrams (main elements over SiO_2). The x-axes (SiO_2) are predefined from 35 to 75 wt. %.
Fenner diagrams	**N**	1 figure with the Fenner variation diagrams (main elements over MgO). The x-axes (MgO) are predefined from axis 0 – 16 wt. %.
K_2O vs. Na_2O	**N**	1 figure with the subdivision of the alkaline series using K_2O versus Na_2O after Middlemost (1975).
AFM diagram	**N**	1 figure to subdivide the subalkaline series into the tholeiitic and calc-alkali series using A (Na_2O + K_2O), F (FeO_{total}) and M (MgO) after Irvine and Baragar (1971).
Mullen (1983)	**N**	1 figure to discriminate the tectonic setting of basalts using TiO_2, MnO, and P_2O_5 after Mullen (1983).

Abbreviations: M = molar data, N = normalized data, R = raw data, S = statistical data.

Tab. 1: (continued).

Button Name	Data	Description
Pearce et al. (1975)	**N**	1 figure to discriminate between oceanic and non-oceanic basalts using TiO_2, K_2O and P_2O_5 after Pearce et al. (1975).
Pearce et al. (1977)	**N**	1 figure to discriminate the tectonic setting of basalts using MgO, FeO_{total} and Al_2O_3 after Pearce et al (1977).
Winchester & Floyd (1977)	**N**	3 figures with the classification diagrams for volcanic rocks (SiO_2 vs. Zr/TiO_2 diagram, SiO_2 vs. Nb/Y diagram and Zr/TiO_2 vs. Nb/Y diagram) after Winchester & Floyd (1977).
Th vs. Co after Hastie et al. (2007)	**N**	1 figure with the classification diagram of altered subduction related volcanic rocks using Th vs. Co as an immobile proxy for K_2O and silica after Hastie et al. (2007).
Condie (2005) Plots	**N**	2 figures using high field strength element ratios (Zr/Nb vs. Nb/Th and Nb/Y vs. Zr/Y) from Condie (2005) and the ΔNb line from Fitton et al. (1997).
Trace elements vs. SiO_2	**N**	6 figures with all trace element variations diagrams over SiO_2. The x-axes (SiO_2) are predefined from 35 to 75 wt. %.
Trace elements vs. MgO	**N**	6 figures with all trace element variations diagrams over MgO. The x-axes (MgO) are predefined from axis 0 – 16 wt. %.
Pearce et al. (1984)	**N**	4 figures with the tectonic discrimination diagrams for granitoids using Rb, Y, Nb, Ta and Yb after Pearce et al. (1984).
Nb-Zr-Y ratios	**R**	6 figures with ratios of Nb, Zr, and Y in different configurations with predefined lines for ratios of 0.2, 1 and 5. Axes are also predefined.
Th-Ta-Hf ratios	**R**	6 figures with ratios of Th, Ta and Hf in different configurations with predefined lines for ratios of 0.2, 1 and 5. Axes are also predefined.
Geotectonic plots	**N**	6 figures with all geotectonic classification diagrams for basalts using trace elements.
Meschede (1986)	**N**	1 figure with the geotectonic discrimination diagram for basalts using Y, Nb and Zr after Meschede (1986).
Pearce & Cann (1973)	**N**	3 figures with discrimination diagrams for basalts (Ti-Zr-Y triangle, Ti-Zr-Sr triangle and Ti vs. Zr linear) after Pearce & Cann (1973).

Abbreviations: M = molar data, N = normalized data, R = raw data, S = statistical data.

Tab. 1: (continued).

Wood (1980)	**N**	1 figure with the discrimination diagram for basalts using Th, Ta, and Hf after Wood (1980).
Cabanis & Lecolle (1989)	**N**	1 figure with the discrimination diagram for basalts using Y, Nb, and La after Cabanis & Lecolle (1989).
REE diagram	**R**	5 figures with rare earth element (REE) pattern normalized to C1-chondrite, primitive mantle, normal mid-ocean ridge basalt, enriched mid-ocean ridge basalt and oceanic island basalt. Normalizing values are taken from Sun & McDonough (1989).
Spider diagram	**R**	5 figures with trace element pattern sorted from incompatible and compatible elements normalized to C1-chondrite, primitive mantle, normal mid-ocean ridge basalt, enriched mid-ocean ridge basalt, and oceanic island basalt. Normalizing values are taken from Sun & McDonough (1989).
Open tables	**R+N**	Open tables with raw data and normalized data for each dataset. Number of figures depends on the number of datasets.
Send tables to Excel	**R+N**	Send tables with normalized dataset to a new tab in the original Excel file. Please close the Excel file before! The export might need some time!
Open statistics	**S**	Open tables with statistics for raw data and normalized data for each dataset. Number of figures depends on the number of datasets.
Send statistics to Excel	**S**	Send tables with statistics of the raw data and normalized data to new tabs in the original Excel file. Please close the Excel file before! The export might need some time!
Open molar tables	**M+S**	Open tables with molar data (in molar per cent) for each dataset. Number of figures depends on the number of datasets.
Send molar tables to Excel	**M+S**	Send tables with molar data and molar statistics to new tabs in the original Excel file. Please close the Excel file before! The export might need some time!
Legend	**-**	Open a separate figure with the legend of current dataset/ datasets.
LOI	**R**	6 figures illustrating the effects of volatile free normalization. Several predefined lines are integrated for comparison.

Abbreviations: M = molar data, N = normalized data, R = raw data, S = statistical data.

Tab. 1: (continued).

M/T	**R**	2 figures showing illustrating the contents of main elements compared to contents of trace elements.
PLOT-O-MAT	**N**	Close FastGAPP and start the PLOT-O-MAT for interactive exploration of the data in linear, semi-logarithmic, logarithmic and triangle plots.
Restart FastGAPP	**-**	Clear all data and go back to FastGAPP initialization window to load new datasets.
Close FastGAPP	**-**	Clear all data and close FastGAPP.
Blank buttons	**-**	These buttons are integrated for future extension and further developments of FastGAPP. They will only open a reminder.

Abbreviations: M = molar data, N = normalized data, R = raw data, S = statistical data.

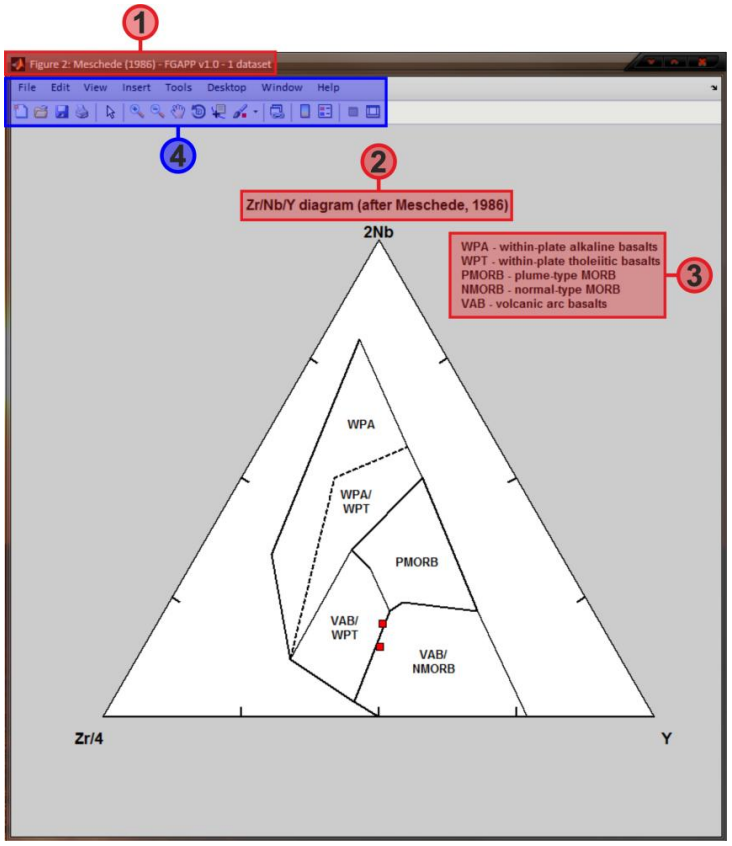

Fig. 9: Example for a final plot in FastGAPP with the two tholeiitic basalts from Riefstahl et al. (submitted). The header of the new figure (1) is always labeled. If a reference was used for any plot it is given over the plot (2). If required, a key of abbreviations (3) is also given near the plot. With the controls of MATLAB it is possible to print, customize or export any of the plots (see chapter 5).

3.7 Displaying data with the PLOT-O-MAT

The PLOT-O-MAT (Fig. 10) is a powerful function integrated in FastGAPP. By a click on the button in the main window (Fig. 8), FastGAPP will close and the PLOT-O-MAT will open and enable to solute the same formula for each axis on the right. The formula is as follows:

$$\frac{\boldsymbol{factor\ 1.1 * factor\ 1.2 * element/oxide\ 1}}{\boldsymbol{factor\ 2.1 * factor\ 2.2 * element/oxide\ 2}} = \boldsymbol{value\ of\ each\ axis}$$

After clicking the “Plot it!!!” button (Fig. 10), the resulting values are calculated and plotted into the chosen diagram type (a linear, semi logarithmic, logarithmic or ternary plot). After having solved the formula for each axis it is possible to choose if the data should be displayed. Note that the z-axis is only needed for ternary diagrams.

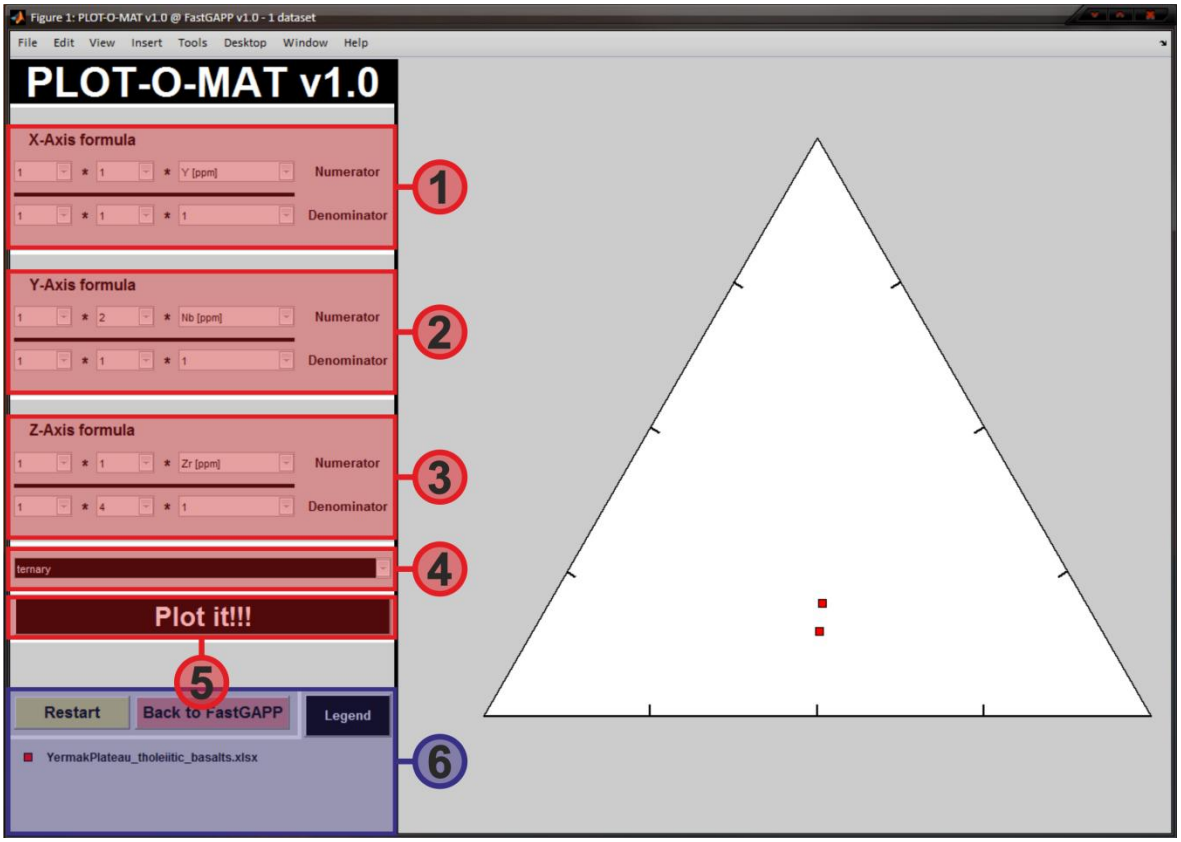

Fig. 10: Screenshot of the PLOT-O-MAT. In this example the ternary Y-2Nb-Zr/4 diagram (Fig. 9) of Meschede (1986) is replicated to illustrate the functionality. Therefore, the formulas of all three axes have been solved with Yttrium on the x-axis (1), Niobium multiplied by 2 on the y-axis (2), and Zirconium divided by 4 on the z-axis (3). Logically, a ternary diagram has been chosen (4) and the “Plot it!!!” button (5) has been pressed to plot the results finally. In the lower left corner (6) it is possible to restart the PLOT-O-MAT, to go back to FastGAPP or to open the legend.

3.8 Comparison of datasets

With FastGAPP it is also possible to plot and compare more than only one geochemical dataset. To plot more than one dataset (two, three or four datasets) it is essential to choose more than one in the FastGAPP initialization window (Fig. 6). To enable the import of more files, the file selection window will be opened again as many times as datasets are chosen. Note that the first dataset that is chosen builds the uppermost layer of the final plot. The first dataset is always displayed as red squares, the second dataset as blue circles, the third dataset as inverted green triangles and the fourth dataset as yellow triangles (Fig. 11).

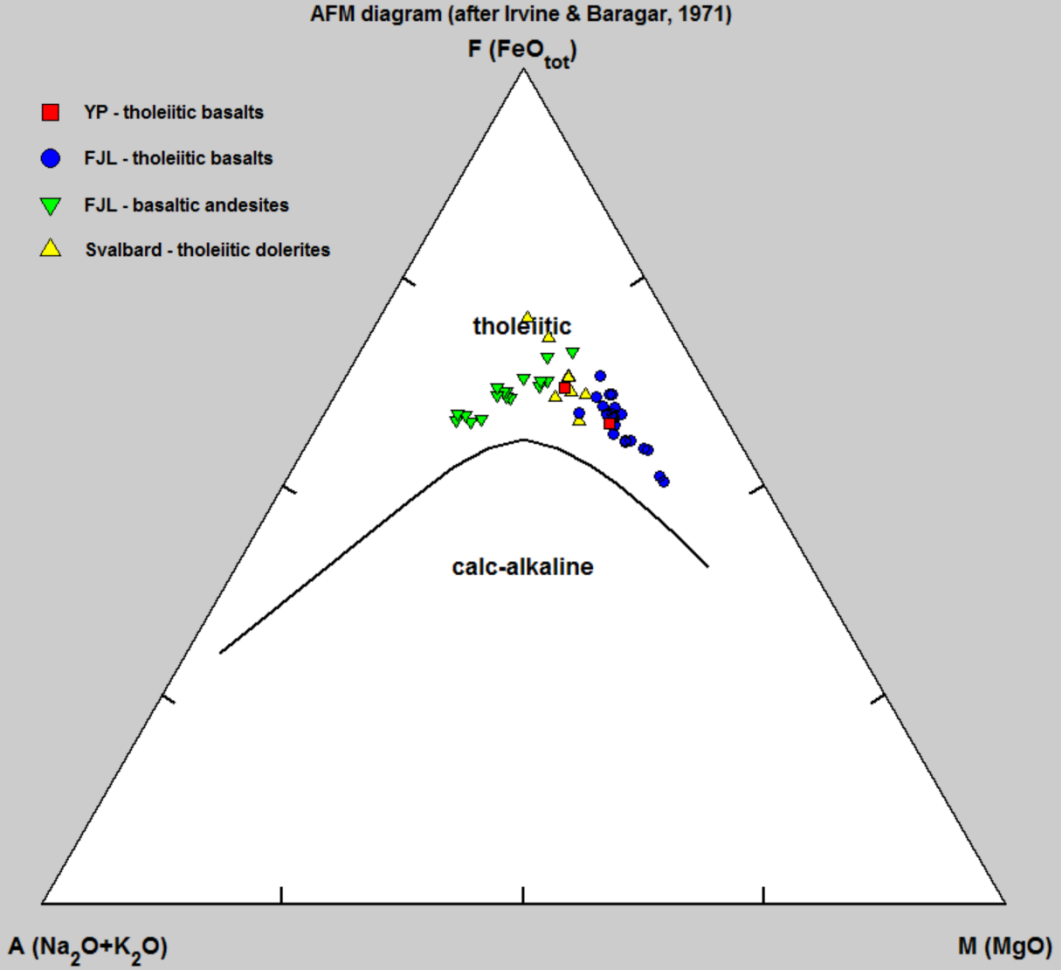

Fig. 11: Example to illustrate displaying of more datasets. In this example, FastGAPP has loaded four datasets plotted into the AFM diagram after Irvine & Baragar (1971). The first dataset contains the two tholeiitic basalts from the Yermak Plateau (YP, Riefstahl et al., submitted) and is displayed as red squares. The second (blue circles) and the third dataset (green inverted triangles) are tholeiitic basalts and basaltic andesites from Franz Josef Land (FJL, Ntaflos and Richter, 2003) and form the middle layers of the plot. For the lowermost layer tholeiitic dolerites from Svalbard (Nejbert et al., 2011) are displayed as yellow triangles. The legend has been created with the legend button.

4. Petro Plot

Petro Plot is a function that contains four different plots (the QAPF classification diagrams for volcanic and plutonic rocks, the triangle classification diagram for mafic gabbroic rocks and the triangle classification diagram for ultramafic rocks). Petro Plot allows plotting and displaying of observed mineral contents from petrographic microscopy of thin sections.

4.1 Preparation of the input for Petro Plot

The three input forms for Petro Plot are stored in the folder *C:\FGAPP\input_forms* as write-protected files in xlsx- and xls-format (e.g. PP_InputForm_QAPF.xlsx for volcanic and plutonic rocks, PP_InputForm_MaficRocks.xlsx for mafic rocks and PP_InputForm_UltramaficRocks.xlsx for ultramafic rocks). First open one of them and second save it with a different name to any folder or use to the predefined folder *C:\FGAPP\petroplot\petrographic_data* (recommended).

Compared to the input form of FastGAPP, the input forms for Petro Plot are very simple and contain only up to 5 columns (for the QAPF diagrams, see Fig. 12). However, the first column is always reserved for the sample number (Numerical values for the sample number will lead to errors!). Put in the results from thin section analyses, make sure that the data are in the right columns and then save it again. Now the file is finally prepared for Petro Plot.

4.2 Starting and using Petro Plot

Open MATLAB and change the current directory to *C:\FGAPP*. After that, start FastGAPP by typing *fgapp* and pressing *enter*. Click on the Petro Plot button on the upper right side of the initialization window (see Fig. 6) to start Petro Plot. After that, choose which diagram to display and select the file for plotting in the next window (Fig. 13). Now a new figure will open and display the selected plot with the chosen data (Fig. 14 and Fig. 15). Note that you have to use the same input form for the same diagram.

	A	B	C	D	E	F	G	H	I	J
1		QAPF - Input					Q = quartz			
2	Sample	Q	A	P	F		A = kalifeldspar (including albite An0 - An5)			
3	xxx	49	31	15			P = plagioclase (An5 - An100)			
4	xxx	45	25	11			F = foides			
5	xxx	42	27	12						
6	xxx	43	22	17						

Fig. 12: Screenshot of a fictive example for petrographic data. The data is accurately prepared for plotting into the QAPF diagram (volcanic or plutonic rocks) with Petro Plot. Note that numerical values for the sample label lead to errors! Please do not put quartz and foides in one line! If there is none of them in a sample, then leave the cell blank as shown in this example!

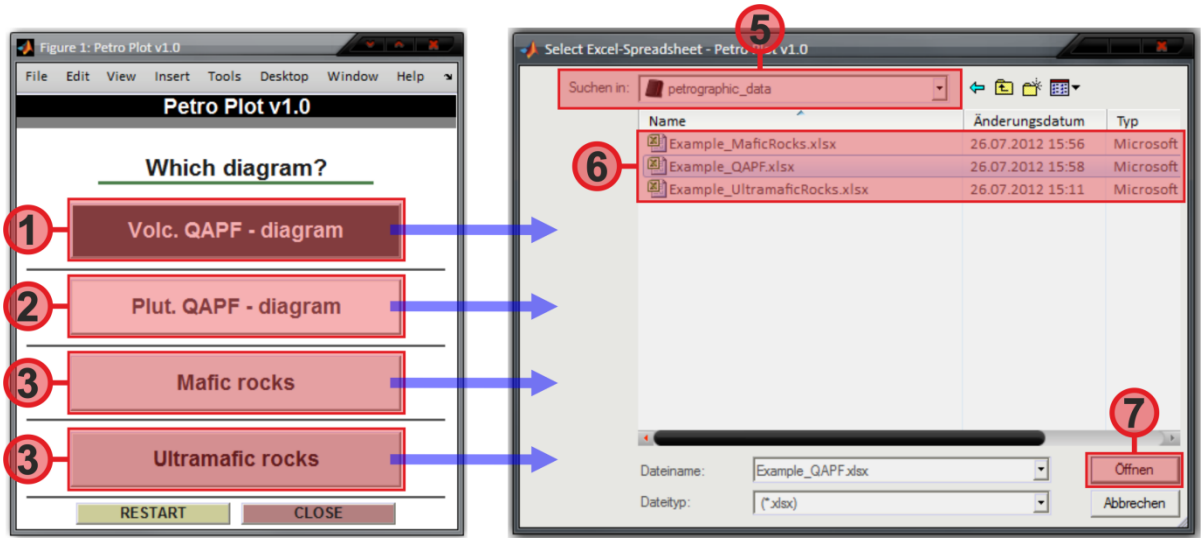

Fig. 13: Screenshots of Petro Plot (left side) and the window for file selection (right side). After starting of Petro Plot choose which diagram should be displayed. The QAPF diagrams for volcanic (1) and plutonic (2) rocks, the triangle for mafic gabbroic rocks (3) and the triangle for ultramafic rocks (4) are contained in Petro Plot v1.0. After having chosen the diagram, a context menu for selection of file opens. Select a folder (5), choose a file (6) and open it (7).

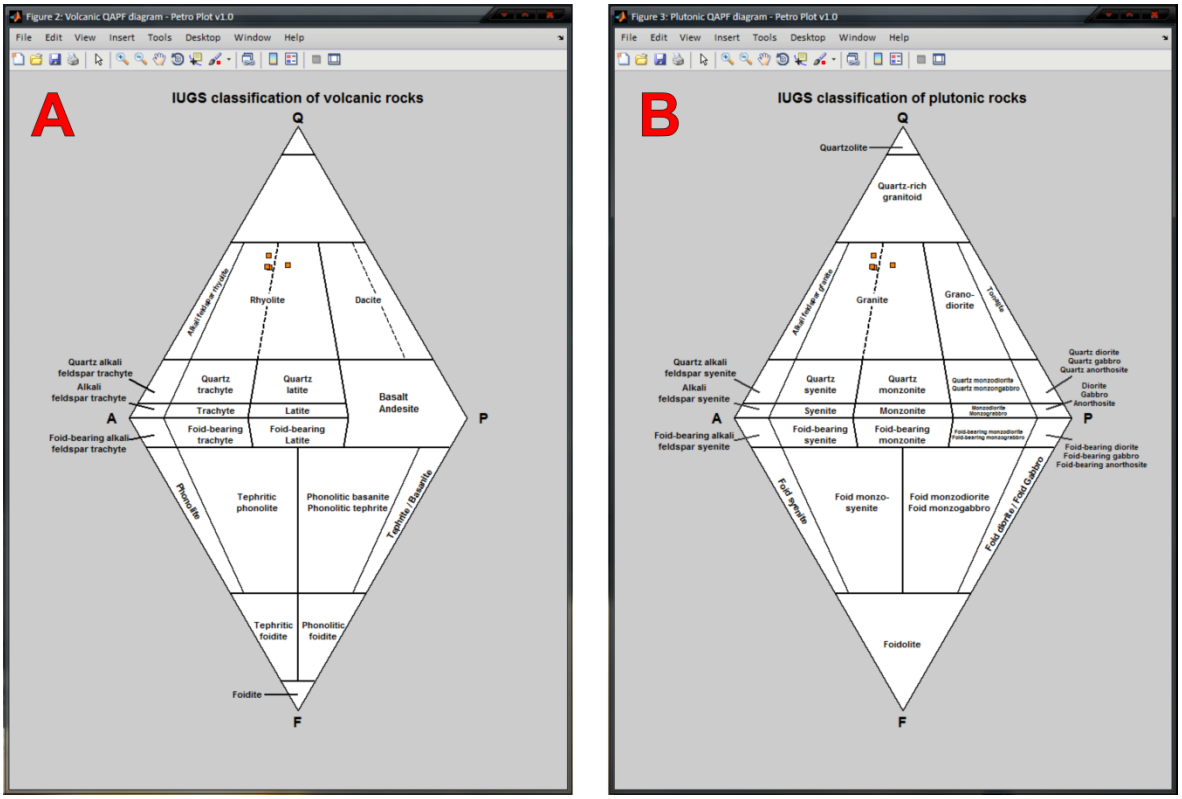

Fig. 14: Screenshots of the diamond diagrams (QAPF) created with Petro Plot. The two diagrams are digitized from recommended IUGS diagrams. A = Classification of volcanic rocks and B = Classification of plutonic rocks. Abbreviations: A = alkali feldspar, F = foides, P = plagioclase, Q = quartz.

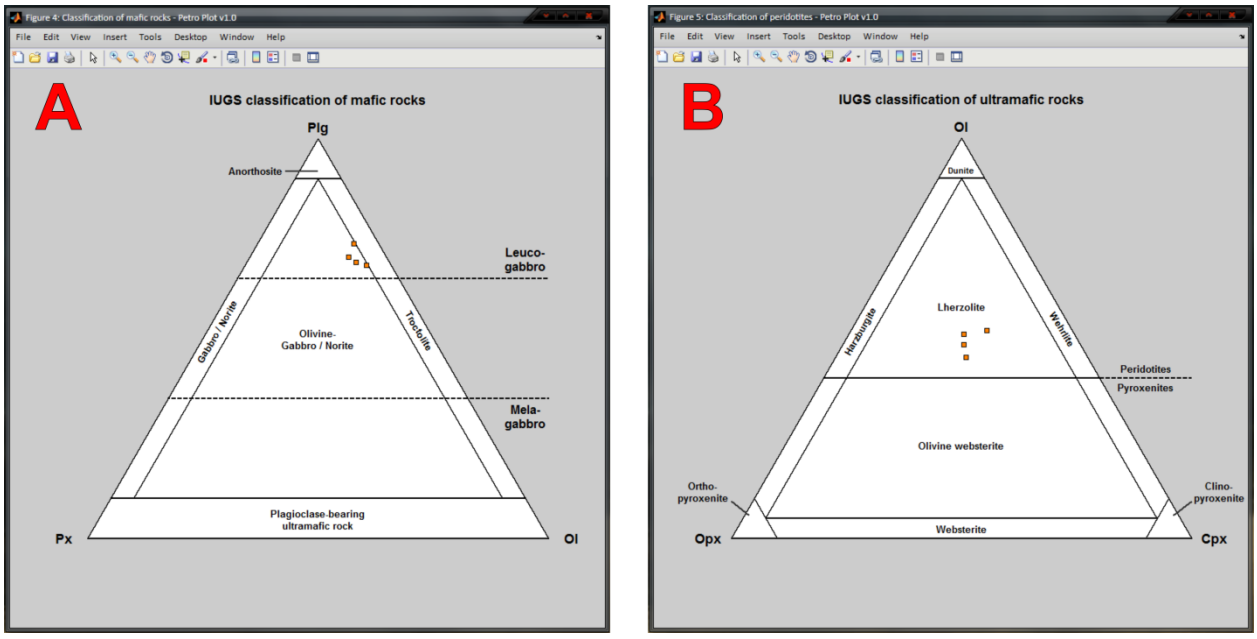

Fig. 15: Screenshots of the triangle diagrams created with Petro Plot. The two diagrams are digitized from recommended IUGS diagrams. A = Classification of mafic gabbroic rocks and B = Classification of ultramafic rocks. Abbreviations: Cpx = clinopyroxene, Ol = olivine, Opx = orthopyroxene, Plg = plagioclase, Px = pyroxene.

5. Export of the plots

To export a final plot, click on “File” in the control elements of the figure (Fig. 16) and after that click on “Export Setup…” to open a new window with export options. In the export options it is possible to change line thicknesses, font sizes, define a custom renderer and the resolution for the final image (e.g. vector format or bitmap format). To save time it is recommended storing the preferred output style and load it again if needed. By a click on “export…”, again a new window will open which allows choosing the export format and file name. Finally click on “save” to create the image.

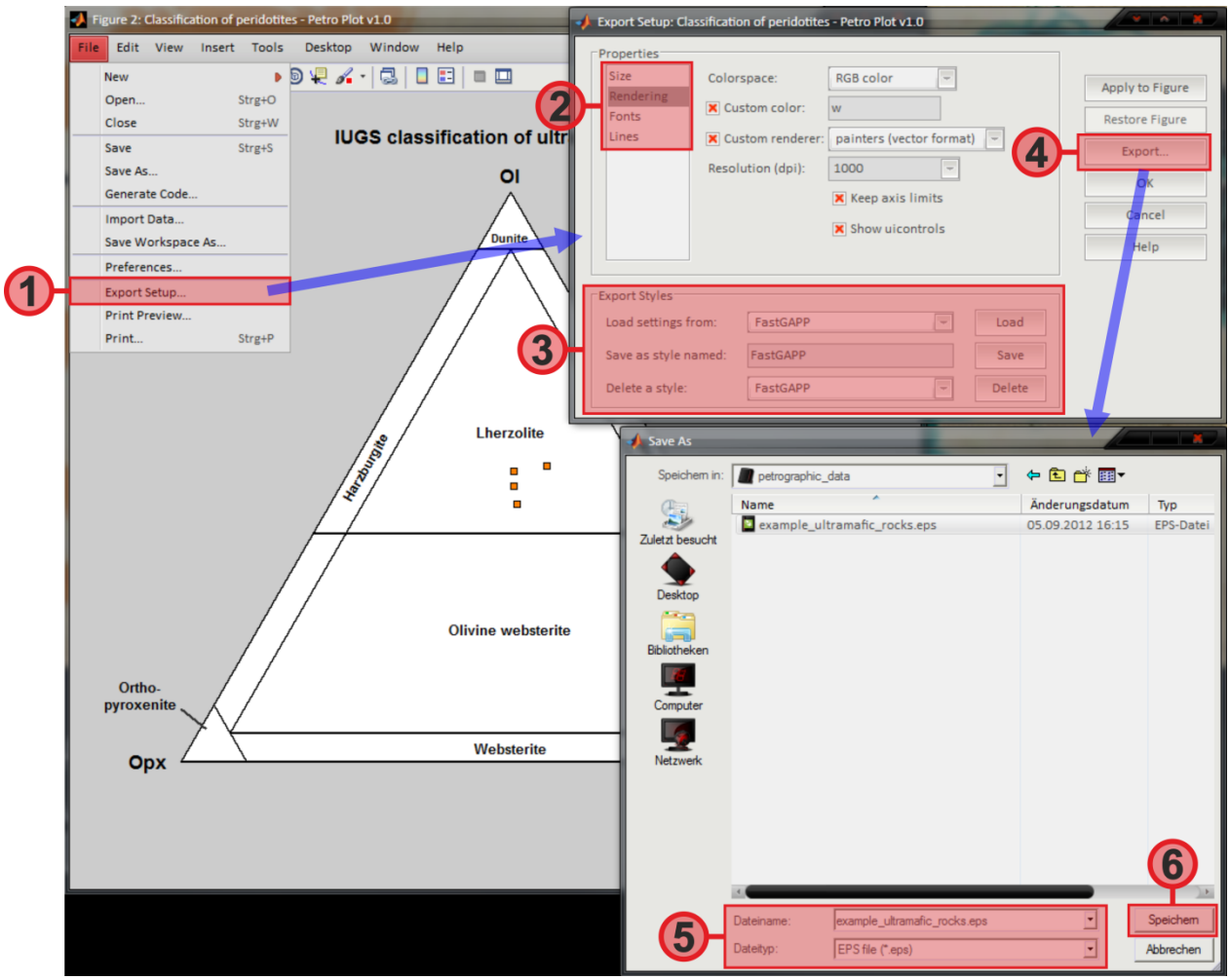

Fig. 16: Screenshot to illustrate how to export an image. First click on “file” in the MATLAB control elements and then click on “Export Setup…” (1) to open the MATLAB image export options. In these options it is possible to change details like the size of the figure, the renderer, fonts, font sizes and the thickness of lines (2). The settings can be predefined and loaded to save time (3). By a click on “Export…”, a new window opens and enables to specify the export format and file name (5). A final click on “Save” will result in the export of the image with the specified settings. MATLAB supports many established file formats (e.g. .emf, .eps, .pdf, .jpg, .png, .tif).

6. External functions

One function (*uibutton*) was downloaded from the MATLAB file exchange and integrated in FastGAPP to gain more control on the button labels. Thanks to Douglas Schwarz to make this useful function available on MATLAB file exchange.
Link: http://www.mathworks.com/matlabcentral/fileexchange/

7. Problems?

If there are any problems running FastGAPP, then write me an Email or join the support group on Facebook.
Email: flo_rief@uni-bremen.de
Facebook: http://www.facebook.com/groups/fastgapp.support/

8. Acknowledgements

First, I want to thank Boris Priehs for the very helpful MATLAB introductions and support during programming FastGAPP.

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Additional thanks to my sister Mirja Riefstahl for the correction of this manual.

9. Glossary

The created variables and used MATLAB functions are listed in the next subchapters to give a short description and overview about the contents of these variables and functions.

9.1.1 Dataset independent variables

folder_norm - folder for normalization scripts
folder_plot - folder for plotting scripts
folder_prog - FastGAPP highest level folder

9.1.2 Dataset specific variables

Note that for the second, third and fourth dataset, the one is replaced by a two, three, or four!

input_comments1 - comments columns from dataset
input_dat1 - numeric raw values from dataset (double array)
input_file1 - name of the first file
input_header1 - header line of the first dataset
input_norm1n - normalization script for the first dataset
input_path_file1 - combined path and file of the first dataset
input_raw1 - raw dataset (cell array)
input_raw_stat1 - contains input statistics of the first dataset
input_samples1 - sample labels of the first dataset
output_molar1 - calculated molar data
output_molar_stat1 - statistics for molar data
output_norm1 - normalized data
output_norm_stat1 - statistics for normalized data

9.2 Geochemical data variables

Note that the different datasets, raw, normalized, and molar data have different prefixes (n1, r1, x1, n2, r2, x2…)! For example n1SiO2 are the normalized silica contents of the first dataset or r2Ag are the raw silver contents of the second dataset.

Ag	- silver	Hf	- hafnium	Rh	- rhodium
Al2O3	- alumina	Hg	- mercury	Ru	- ruthenium
As	- arsenic	Ho	- holmium	SO3	- sulfur trioxide
Au	- gold	In	- indium	Sb	- antimony
B	- boron	Ir	- iridium	Sc	- scandium
Ba	- barium	K2O	- potassium oxide	Se	- selenium
Be	- beryllium	LOI	- loss on ignition	SiO2	- silica
Bi	- bismuth	La	- lanthanum	Sm	- samarium
CO2	- carbon dioxide	Li	- lithium	Sn	- tin
CaO	- calcium dioxide	Lu	- lutetium	Sr	- strontium
Cd	- cadmium	MgO	- magnesia	Ta	- tantalum
Ce	- cerium	MnO	- manganese oxide	Tb	- terbium
Cl	- chlorine	Mo	- molybdenum	Te	- tellurium
Cr	- chromium	Na2O	- sodium oxide	Th	- thorium
Cs	- cesium	Nb	- niobium	TiO2	- titania
Cu	- copper	Ni	- nickel	Tl	- thallium
Dy	- dysprosium	Os	- osmium	Tm	- thulium
Er	- erbium	P2O5	- phosphorus oxide	U	- uranium
F	- fluorine	Pb	- leak	V	- vanadium
Fe2O3	- total iron	Pd	- palladium	W	- tungsten
Ga	- gallium	Pr	- promethium	Y	- yttrium
Gd	- gadolinium	Pt	- platinum	Yb	- ytterbium
Ge	- germanium	Rb	- rubidium	Zn	- zinc
H2O	- water	Re	- rhenium	Zr	- zirconium

9.3 Total values

Note that the different datasets, raw, normalized and molar data have different prefixes (n1, r1, x1, n2, r2, x2…)!

n1total	- normalized total value (should be 100 wt. %)
r1total	- sum of all elements without LOI
r1totalLOI	- sum of all elements including LOI
r1totalLOImain	- sum of main elements and LOI
r1totalinput	- input total value
r1totalmain	- sum of main elements without LOI
x1sum	- molar total value (should be 100 wt. %)

9.4 MATLAB commands used for FastGAPP

axes - create a new axes object
axis - axis scaling and appearance
box on - switch axes border on
box off - switch axes border off
cat - concatenate array along specific dimensions
cd .. - one level up from current folder
cd(x) - change current folder to x
cell2mat - convert cell array to single matrix
clc - clear command window
clear - clear a variable
close - close specific figure
cot - cotangent of argument in radians
datestr - convert date and time to string format
deg2rad - convert angles from degree to radians
evalin - execute MATLAB expression in specific workspace
figure - create a new figure
hold - retain current graph in figure
isnan - determine whether array elements are NaN
isfinite - determine whether array elements are finite
line - create line object (slightly similar to plot)
loglog - log-log scale plot
max - largest elements in array
mean - average or mean value of array
min - smallest elements in array
movegui - move GUI figure to specified location on screen
ones - create array of all ones
patch - create a filled polygon
plot - 2 dimensional line plot
pwd - identify current folder
run - run script that is not in the current folder
set - set properties of graphics object
semilogx - semi-log x-axis plot
semilogy - semi-log y-axis plot
sin - sine of argument in radians
size - returns array dimensions
sprintf - format data into string
subplot - create axes in tiled positions
sum - sum of array elements
text - create text object in current axes
tic/toc - start/stop clock
uibutton - create a GUI control object with more text properties
uicontrol - create a GUI control object
uitable - create a GUI table object
uigetfile - open standard dialog box for retrieving files
xlabel - label x-axis
xlim - set or query x-axis limits
xlsread - read MS Excel spreadsheet file
xlswrite - write MS Excel spreadsheet file
ylabel - label y-axis
ylim - set or query y-axis limits
zeros - create array of all zeros

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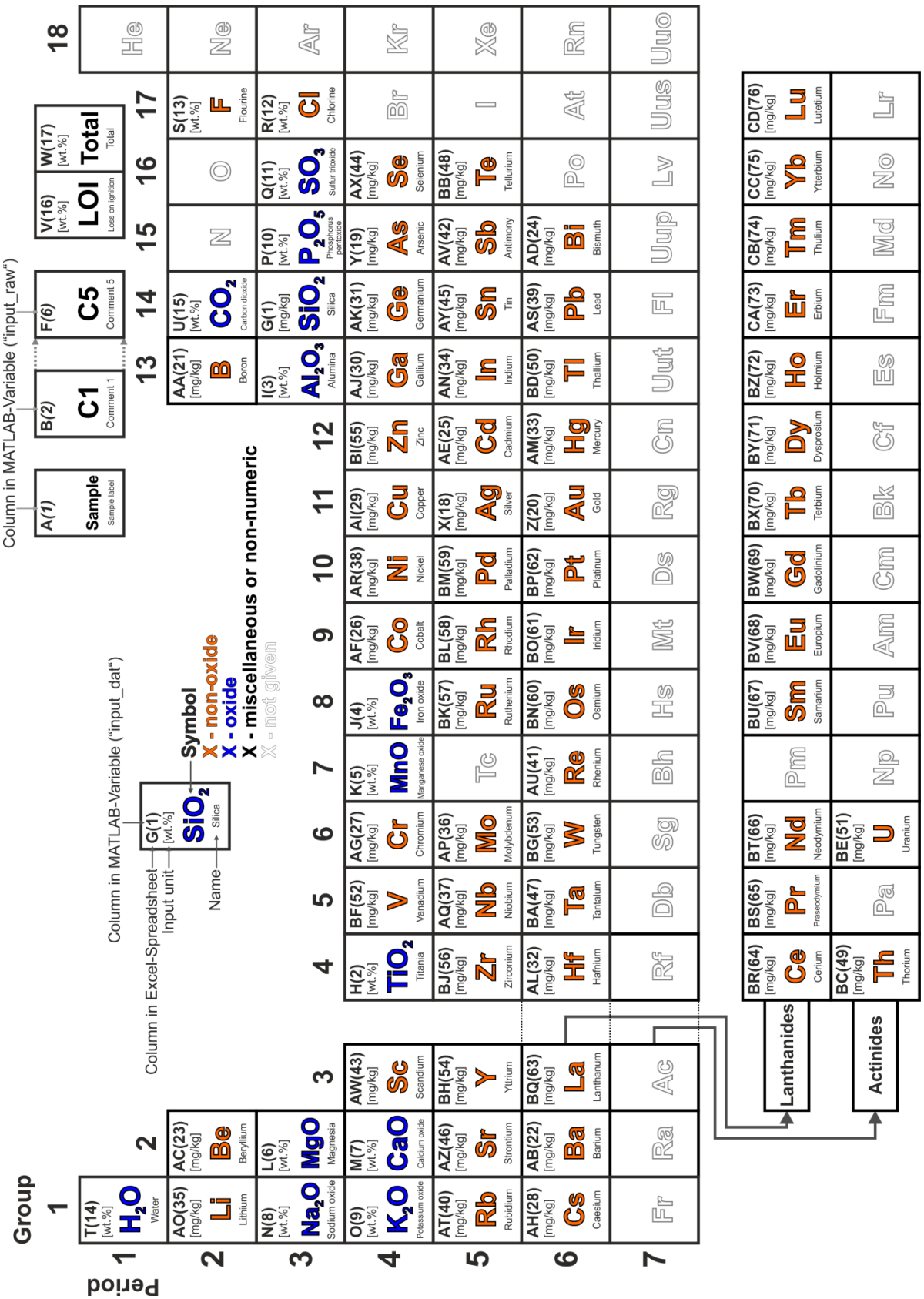
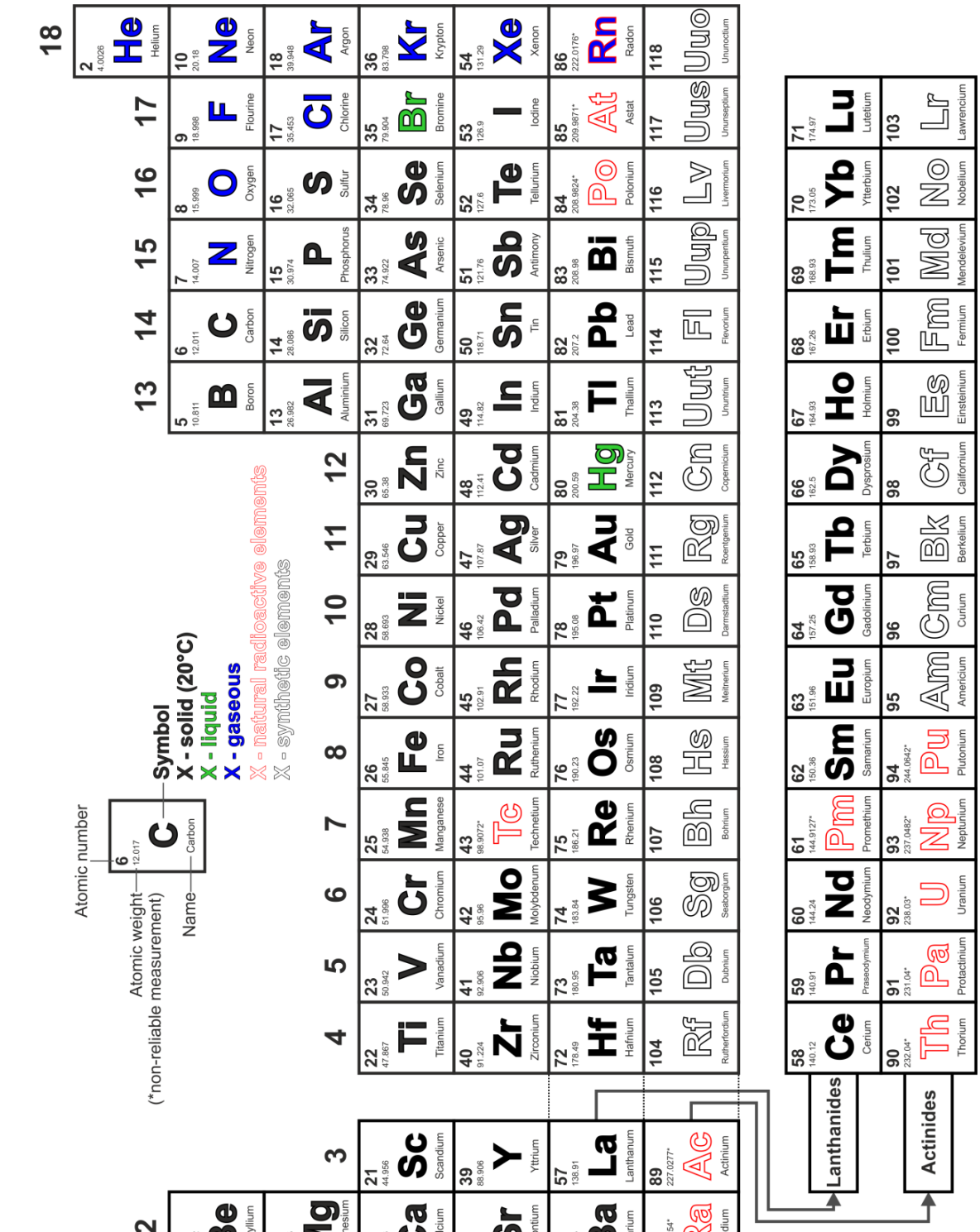
Appendix 1



Appendix 1: Periodic table of elements and oxides with column in Excel spreadsheet and MATLAB input variables.

Appendix 2



Appendix 2: Periodic table of elements with recommended atomic weights of each element from the International Union of Pure and Applied Chemistry (IUPAC).