

Geochemical Data Toolkit (GCDkit): a Key for Magmatic Geochemists to the Treasury of Data Analysis, Statistics and Graphics in R

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The need to quantify aspects of the world in which we live is inherent in contemporary scientific thinking. Magmatic geochemistry is no exception, inasmuch as there is often no first-hand experience with the studied phenomena. Such an approach leads inevitably to a flood of numeric data, which have to be analysed by an appropriate and potent software tool.

In our view this has to have several features: (1) perform commonly used petrochemical re-calculations and straightforward data handling, (2) offer flexible and high-level graphical functions with an output into a widely used vector format, (3) allow additional calculations and statistical analysis when necessary, (4) avoid any licensing problems. As there is strong demand for such software, several programs have been released, such as MinCalc (Melin and Kunst, 1992), Newpet (Clarke, 1993), MinPet 2 (Richard, 1995), IgPet 2000 (Carr and Dehn, 2003), Norman (Janoušek, 2000) or various MS Excel plug-ins. However, none of these products meets all the above mentioned requirements. Geochemical Data Toolkit for R (GCDkit) is our response to this challenge.

GCDkit is a tool for whole-rock magmatic geochemistry built using R, an environment for data analysis and graphics (Ihaka and Gentleman, 1996). R is available publicly under the terms of the Free Software Foundation's GNU General Public License, and can be downloaded from www.r-project.org. The user communicates mainly via the command line, but includes functions for facilitating Windows-like interaction (GUI=graphical user interface) and these are exploited by the GCDkit.

GCDkit not only provides a user interface to the powerful functions built in R, but also adds on specialized tools for handling and recalculation of whole-rock major- and trace-element analyses and Sr–Nd isotopic data from igneous rocks. All functions are accessible via pull-down menus, as well as in the interactive regime.

When a tab-delimited data set is loaded into the system, all metadata (i.e., non-numeric strings) are stored in a data frame 'labels' whereas numerical data are allocated into a matrix 'WR'. Additionally, all missing data are replaced with the NA (= not available) values, and some additional parameters are calculated (anhydrous major-element data and millifications), and, if necessary, columns with some commonly used geochemical indexes are appended to the matrix 'WR' (mg#, FeO_t,

A/CNK etc). Subsequently, operations available to the user can be split into several categories:

- **Data handling**, including generation of subsets, sorting into groups on the basis of various criteria, direct editing of the data or adding new variables (columns). The data searches and creation of subsets is performed using conditions employing regular expressions and Boolean logic. Important feature of data handling in the GCDkit is grouping. All analyses may be sorted into unique groups, which are subsequently utilized by some statistical and plotting functions (and as a factor by power users). Groups can be assigned on the basis of labels (locality, rock type ...), a value of a chosen numerical variable, position in classification diagram (e.g., TAS) or cluster analysis. The grouping information is stored in vector 'groups' until the next assignment is performed.
- **Basic descriptive statistics**, including histograms, box-and-whiskers diagrams, correlation plots, principal components or cluster analysis. Each of the implemented functions is also equipped with a powerful data filter to specify the data that are to be processed.
- **Plotting functions**, including user-defined binary or ternary plots, coplots, as well as Harker diagrams, spiderplots or variable visualisations of Sr–Nd isotopic data. A wide palette of classification and geotectonic discrimination diagrams is available, and new templates can be added in a rather simple way. All plots are publication-ready, however, if need be, the graphic output may be saved in Postscript or Windows Metafile (WMF) and further embellished in any vector-based drawing program.
- **Figaro** – a set of interactive tools for editing and annotation of all classification and some geotectonic diagrams (zooming, editing axis labels, adding comments or legend, identifying points and many others)
- **Recalculation algorithms**, such as CIPW, Catanorm, Granite Mesonorm, Niggli's numbers, as well as variable saturation calculations (apatite, zircon and monazite).

To sum up, the GCDkit is software written by geochemists for geochemists that grew continually in response to authors' everyday needs. Thus, it was designed to eliminate routine and tedious operations involving large collections of whole-rock data

and, at the same time, to make accessible a wealth of statistical functions built into R. Nevertheless the main aim was to free the igneous geochemists for inventive thinking.

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Composition of Fluids and their Effect on Stability Fields of Silicate Minerals in Amphibolite Facies Metamorphic Rocks

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Mineral reactions and petrological properties of rocks critically depend on the presence and composition of fluids during metamorphism. Fluid inclusions and phase equilibria from most amphibolite/granulite facies rocks indicate the presence of low water activity fluids. This is confirmed in the whiteschist locality of Sare Sang (Afghanistan), where metamorphic minerals with structural CO₂, H₂O, halogens, sulfur and boron are widespread. The host rocks of these minerals are marbles, different varieties of calc-silicate rocks and whiteschists. Sedimentary origin of these rocks as well as of CO₂ and brines is also supported by stratigraphic control of the occurrence of carbonate and Na-, Al- or Mg-rich minerals that follow bedding in the Sare Sang Series. The origin of calc-silicates and whiteschists is connected with the occurrence of carbonate-evaporite layers within psammopelitic rocks. Textural relations and mineral compositions indicate a high-pressure amphibolite facies metamorphism with various stages of retrogression. The main volatile-bearing phases in the rocks are carbonates, sodalite-group minerals, scapolite, amphibole and biotite. However, most of these minerals have retrograde origin. Minerals stable at peak P-T conditions were carbonates, graphite, scapolite, apatite, amphibole, phlogopite, talc, clinohumite, pyrrhotite and pentlandite. Low water activity of fluids during metamorphism is documented by high X_{Cl}

and X_F content in amphibole and biotite as well as by the presence of sodalite and fluorapatite veins in the rocks. Besides lithology, variation of volatiles in minerals was controlled by avoidance criteria of elements in mineral structure. The high F or Cl contents led to the stability of F-phlogopite, Cl-biotite and Fe (Cl)- amphibole. Calculated log (X_F/X_{OH}) and log (X_{Cl}/X_{OH}) in coexisting biotite and amphibole indicate preferential partitioning of Cl into amphibole and F into biotite. Chlorine enters biotite and amphibole structure by factor near 1:1. However, F indicates preferential partitioning by factor of 9:4. F-OH and Cl-OH partitioning coefficients for apatites showed preferential entering of F into apatite relative to biotite. The degree of preference depends on temperature and Fe concentration in biotite. The retrogression that was accompanied by granite formation led to recrystallization of these minerals as well as to fluid infiltration and metasomatic reactions in the surrounding rocks. The crystallization of numerous minor discordant intrusions of post-metamorphic granite would have released water, which permeated through the carbonate-evaporite sequence having enriched it with S, Cl and CO₂. These processes led to formation of the main lapis-lazuli deposit in the Sare Sang locality. The best evidence of this model is the accumulation of lapis lazuli near the granite contact.