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Interpretation of geochemical data from magmatic rock suites using the R language – the current state of play

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With the appearance of R (Ihaka & Gentleman, 1995; *www.r-project.org*) at the turn of millennium, the scientists were given a powerful, yet simple and versatile, open-source toolbox. The R language represents an ideal environment for development of packages for interpretation of often extensive and complex data sets in virtually any field of the human activity. One of these user-added packages, the Geochemical Data Toolkit (*GCDkit*, *www.gcdkit.org*), dedicated to graphical presentation and recalculation of data in igneous and metamorphic geochemistry, has been published already ten years ago (Janoušek et al., 2006).

The current version of GCDkit (4.1, aka *Chlopskie jadlo*) has been released in February 2016. The main features include switching between several datasets stored simultaneously in memory, their over plotting and improved capabilities to scripting and running in batch mode. The previous one (4.0, *Great October Revolution*) brought about a namespace (thus minimizing potential clashes with other packages), semitransparency of plotted symbols/fields, a possibility of assigning plotting colours according to values of a numeric variable, new geotectonic diagrams, rutile saturation module and help system with graphics.

Our new textbook (Janoušek et al., 2016) aims to mediate the power of R to anyone dealing with petrogenetic interpretation of magmatic rocks. At beginning, it provides worked examples how to employ R to simple recalculations and plotting of geochemical data. Further it explains fundamentals of numerical modelling of igneous processes, e.g. partial melting, fractional crystallization, binary mixing or AFC using major-, trace-element and radiogenic isotope data. It gives numerous solved exercises illustrating the implementation of these theoretical principles in the plain R and/or *GCDkit*. Lastly, it includes examples indicating how forward/reverse geochemical modelling helps us to understand geological problems, and critically assesses the limitations or possible pitfalls each of these approaches. The concluding sections demonstrate examples of successful modelling strategies applied to the differentiation of arc-related volcanic rocks from Ecuador and progressive melting from the Saint-Malo migmatites in Brittany. The appendices outline the syntax of the R language and provide a quick introduction to the GCDkit.

Current development is directed towards releasing a platform-independent version (a *GCDkit* running on Mac, Linux, or on a server), automated report creation (in Word or Open Office), online connection to web-based databases such as *earthchem.org*, building an interface to popular thermodynamic programmes (e.g., Perplex) and providing simple GIS capabilities.

Ihaka R. & Gentleman R., 1996: R: A language for data analysis and graphics. *Journal of Computational and Graphical Statistics*, 5, 299–344.

Janoušek V., Farrow C.M. & Erban V., 2006: Interpretation of whole-rock geochemical data in igneous geochemistry: introducing Geochemical Data Toolkit (GCDkit). *Journal of Petrology*, 47, 1255–1259.

Janoušek V., Moyen J.F., Martin H., Erban V. & Farrow C.M., 2016: Geochemical Modelling of Igneous Processes – Principles and Recipes in R Language. Springer, Berlin, ISBN 978-3-662-46791-6.