GCDkit: New PC software for interpretation of whole-rock geochemical data from igneous rocks

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The dearth of truly potent and flexible software for recalculation and plotting of whole-rock analyses is often a limiting factor to a creative scientific work in igneous geochemistry. An ideal package should include a variety of calculation schemes, produce publication quality diagrams, be readily available, easy to use and expand. The **Geochemical Data Toolkit** (GCDkit) is being developed to meet this requirement, with facilities for handling and recalculation of whole-rock major- and trace-element as well as Sr–Nd isotopic data. It is built using the freeware R language, version for Windows (*http://www.r-project.org*) which in itself provides a rich environment for data analysis, graphics and software development.

Data management includes loading and saving of free form text files, data editing, searching and generation of subsets using regular expressions and Boolean logic. Analyses may be grouped for subsequent statistical processing or plotting on the basis of particular attributes (locality, rock type…), ranges of a numerical variable, by cluster analysis or using a selected classification diagram (TAS, R_1–R_2…). Statistical functions include simple descriptive statistics, histograms, box-and-whiskers dia-grams, correlation plots, coplots, or multivariate methods such as principal components analysis. Also implemented are recalculation and normative algorithms, for instance CIPW, Catanorm, Granite Mesonorm, Niggli's values, as are the common geochemical plots (e.g. Harker diagrams, AFM, spider diagrams, REE plots). A wide palette of classification and geotectonic diagrams are available, and new templates can be added. All plots are publication ready but can be further retouched (editing axes labels, adding comments or legend, identifying data points).

With the current version are plugin modules to calculate saturation temperatures of various accessories (apatite, zircon and monazite) and for interpretation of the Sr–Nd isotopic data (initial isotopic ratios, Nd model ages, isochron plots and plots involving the isotopic data). Modules for petrogenetic modelling are under development. Users with an understanding of the R language will readily be able to enhance the functionality.