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GCDkit.Mineral: a flexible, platform-independent R package for recalculation and plotting of mineral chemistry data

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Over the years, *Geochemical Data Toolkit (GCDkit)* became an established tool for interpretation of whole-rock geochemical data from igneous and metamorphic rocks [1–2]. To celebrate its 20th birthday [3], we release a new R package *GCDkit.Mineral* – a platform-independent system for handling, recalculation, statistical treatment and plotting of mineral chemistry data obtained by microbeam techniques.

The *GCDkit.Mineral* imports essentially freeform data in a variety of file formats, or retrieves them from clipboard. Available are routines for effortless data management, i.e. searching, subsetting and grouping. The raw (wt.%) chemistries are recalculated to apfu based on fixed number of oxygen equivalents, atoms or charges, with, or without, Fe^{II}/Fe^{III} estimation by a multitude of methods. The apfu are recast to structural formulae, user-defined parameters and/or end-member percentages. The data can be treated statistically, using descriptive and multivariate methods, provided by the lively R community [*http://www.r-project.org*]. The raw and recalculated mineral chemistries can be plotted onto a binary and ternary plots, multiple plots and boxplots. The graphical output can be retouched and exported into a many graphical formats, including (E)PS and PDF. The general classification routine allows to build hierarchical schemes combining binary and ternary diagrams, together with, if need be, external R scripts.

For ordinary users, *GCDkit.Mineral* is fully menu-driven and comes with typical recalculation schemes for many rock-forming minerals. Those more proficient in mineralogy can easily tweak the database of recalculation options. By seasoned R programmers, the *GCDkit.Mineral* can be invoked from the program prompt, external scripts or Python-driven notebooks (project Jupyter). The lucid, open and modular design makes *GCDkit.Mineral* a promising platform for further community-driven software development.

GCDkit-family tools can be downloaded from www.gcdkit.org.
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References

[1] Janoušek, Farrow & Erban (2006), *Journal of Petrology* 47, 1255-1259

[2] Janoušek, Moyen, Erban, Farrow & Martin (2016), *Geochemical Modelling of Igneous Processes – Principles and Recipes in R Language.* Berlin: Springer.

[3] Janoušek, Farrow & Erban (2003), *Geochimica et*