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The Geochemical Data Toolkit (GCDkit) family of tools – a progress report

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During more than 20 years of its existence, our R-language (<https://www.r-project.org>) software Geochemical Data Toolkit (GCDkit; <https://gcdkit.org>) became an established standard in recalculation and plotting of whole-rock geochemical data from igneous and metamorphic rocks.

Only recently, however, was unleashed GCDkit.Mineral (<https://mineral.gcdkit.org>), a much needed package for handling mineral analyses acquired by electron-probe microanalysis. Apart from recalculation to atoms per formula unit (apfu) by a number of methods (with, or without, the Fe²⁺/Fe³⁺ estimation), it yields structural formulae, end-member proportions and, for some mineral groups, provides IMA classification. The calculation options, stored externally, can be easily customized, and new calculation schemes/minerals introduced. Both the raw and recalculated data can be subsequently treated by assorted graphical and statistical tools, complemented by those of the standard GCDkit and R.

But even the aging GCDkit continues to be developed. In January was released version 6.2.0, bringing, among other features, new plugin escoRt implementing the expert system of Pearce (1987) to identify the geodynamic setting of ancient igneous rock suites, and functions to calculate ideal mineral compositions based on extensive database of mineral formulae (Le Maitre 1982). The newest addition represents HafAn, a GCDkit plugin for recalculation, visualization and statistical treatment of in-situ U–Pb ages and Hf isotopic data from igneous and detrital zircons. The debugging and writing documentation are coming to the close, and thus the plugin is due to be released soon.

Underway is also preparation of the second edition of our monograph on numerical modelling of geochemical data in R (Janoušek et al. 2016 – Springer) with envisaged publication in late 2025. The volume will be substantially updated and expanded, including brand new chapters on thermodynamically-based models based on established programs MELTS, Perple_X and Rcrust (Mayne et al. 2016). Among other developments, the text shall introduce also our new package for seamless interaction with the MELTS thermodynamic software (<https://melts.ofm-research.org>), using GCDkit for editing the modelling parameters, as well as plotting and computing complementary trace-element data. Most of the code is ready, and it is currently being optimized for speed, using, inter alia, the powerful tools for parallel R computing.

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