

Quo vadis, GCDkit?

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In igneous geochemistry, we are facing a recent flood of high-precision data – acquired by the advancing analytical techniques as well as coming from literature, experiments and numeric simulations. We need to secure their storage, interoperability, (multivariate) statistical treatment and adequate graphical presentation. Besides that, we crave for potent software to automate labour-intensive tasks and perform geochemical modelling. For some of these tasks, existing programmes, written in various languages, need to be integrated.

The viable solution relies on freely available and portable scientific languages such as R, Python, Julia, or Octave. During two decades of its existence, our R-language Geochemical Data Toolkit (*GCDkit*; <https://gcdkit.org>) [1] became a tool of choice for handling whole-rock geochemical data from igneous and metamorphic rocks. Recently, it was joined by *GCDkit.Mineral*, a package for recalculations and graphical presentation of mineral analyses acquired by microbeam techniques [2].

Both packages can be easily expanded by the so-called plugins. These provide a platform for community-driven geochemical software development or for standard modules requiring special datasets. For instance, the newest addition represents *HafAn*, a *GCDkit* plugin for recalculation, visualization and statistical treatment of *in-situ* U–Pb ages and Lu–Hf isotopic data [3]. Similarly, the *EscoRt* plugin implements the expert system that determines the geodynamic setting of ancient igneous rock suites [4].

The R with *GCDkit* is a great platform for modelling of geochemical data from igneous rocks, integrating the established software tools. The second edition of our monograph on this topic [5] shall be substantially updated and expanded, including new chapters on thermodynamically based models (using MELTS, Perple_X and Rcrust [6]). Among other developments, the text shall introduce our new package for seamless interaction with the MELTS thermodynamic software (<https://melts.ofm-research.org>), using *GCDkit* as a front-end, as well as an environment for plotting and computing complementary trace-element data.

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[1] Janoušek *et al.* (2006) *J. Petrol.* 47, 1255-1259.

[2] Janoušek *et al.* (2024) *Amer. Miner.* 109, 1598-1607.

[3] Janoušek (2024) *J. Geosci.* 69, 151-160.

[4] Pearce (1987) *J. Volcanol. geotherm. Res.* 32, 51-65.

[5] Janoušek *et al.* (2016) Springer.

[6] Mayne *et al.* (2016) *JMG* 34, 663-682.

