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Revision 1

GCDkit.Mineral – a customizable, platform-independent R-language environment for recalculation, plotting and classification of electron-probe micro-analyses of common rock-forming minerals

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ABSTRACT

GCDkit.Mineral is a platform-independent (Windows/Mac/Linux) freeware for recalculation, plotting and statistical treatment of mineral data obtained by microbeam techniques, typically an electron microprobe. It is written in R, a language providing a feature-rich environment for statistics and data visualization.

This new program imports compositional data in a variety of commonly used file formats, or retrieves them from the clipboard. Routines are available for data management, i.e. grouping, searching, and generation of subsets, using regular expressions and Boolean logic. Raw compositional data (wt.%) are recalculated to atoms per formula unit (apfu) based on a required number of O equivalents, atoms or charges, with or without, Fe^{II}/Fe^{III} estimation by a variety of methods. Analyses may then be recast to structural formulae; i.e. the atoms are distributed into appropriate crystallographic sites. For minerals forming solid solutions, the molar percentages of end members are computed. All the data may be treated statistically, either by built-in functions for descriptive and multivariate statistics, or using the wealth of tools provided by the wide R community.

Raw and recalculated mineral data may be plotted on assorted binary and ternary plots, and boxplots. Most are defined as internal templates that provide a means to make later changes to the plot (zooming and scaling, adding comments or legend, identifying data points, altering the size or color of the plotting symbols, etc.). The publication-ready graphics may be saved into a number of vector- (PostScript, PDF and WMF) and bitmap-based (e.g., PNG, TIF and JPG) formats, ready to be imported into a professional graphical, presentation, or desktop publishing software.

Importantly, the graphical templates are used as a basis for classification. The general classification routine looks for the name of the polygon within the diagram (= graphical template), into which the analysis falls according to its x–y coordinates. The outcome may be

either a name of the mineral or a link to another diagram, in the case of more complex classification schemes. Following the rules of the International Mineralogical Association (IMA), in some cases the classification is not done graphically, but using prescribed algorithms.

The class mechanism in R provides an elegant solution to the computational problems presented by the differing requirements of each mineral group. By assigning each mineral species to a particular class, all algorithms may be implemented as mutually independent, but mineral group-specific, methods. The default recalculation options for each mineral class are stored externally in a small and simple text file.

The program is designed to cater for three potential user groups. For users with no familiarity with R, the program is fully menu-driven and contains embedded default recalculation options for many common rock-forming minerals. More experienced users may easily tweak these parameters, as they are saved in a logically structured plain text file. Seasoned R users may invoke *GCDkit.Mineral* in command line mode, use batch scripts or Python-driven notebooks (e.g., of project *Jupyter*), or modify and develop new recalculations or plugins.

The lucid, open, and modular design thus makes *GCDkit.Mineral* a versatile workbench for everyday use as well as a promising platform for community-driven development. The *GCDkit* family of R tools, including *GCDkit.Mineral,* is distributed through the WWW. The current version may be downloaded from http://mineral.gcdkit.org.

INTRODUCTION

Today, petrologists, geochemists and mineralogists alike face a flood of high-quality electron-probe micro-analysis (EPMA) mineral compositional data. Interpretation of these data may

require tedious, mineral-specific recalculations and plotting. First, raw mineral analyses must be recast to atoms per formula unit (apfu) that allow deeper insight into mineral crystal chemistry (e.g., nature and extent of substitutions at each of the crystallographic sites) and serve for mineral classification according to the IMA rules (International Mineralogical Association 2020). Moreover, in the field of igneous and metamorphic petrology and geochemistry, the apfu form a basis for most of the conventional geobarometers and geothermometers (Spear 1994; Putirka 2008; Anderson et al. 2008, 2018). The apfu also facilitate a direct linkage with whole-rock geochemistry-derived parameters (e.g., millications-based ones) useful for rock nomenclature and petrogenetic considerations (De La Roche et al. 1980; Debon and Le Fort 1988; Bonin et al. 2020).

At the same time, there is a dearth of efficient, comprehensive, flexible, and customizable software for recalculation of large mineral compositional data sets. Ideally, such software would be free, platform-independent and developed in a widely used, easy-to-understand programming environment. It should run from a menu-driven interface as well as directly, either interactively (from command prompt) or in batch mode (allowing scripting for automated use). The program should produce high-quality graphical output, ideally publication-ready, and allow statistical treatment of the raw and recalculated data. Lastly, the software should have an open and well-thought architecture, facilitating modifications.

We present our new R-language package, *GCDkit.Mineral,* designed to follow these guidelines. Instead of producing software that incorporates as many recalculation schemes and classification options as possible for each of the main mineral groups – which are subject to change and often a matter of personal preference – we have chosen to design an open platform that could be tailored to the needs of each user and that allows further expansion through community-driven development.

THE NEW R PACKAGE *GCDKIT.MINERAL*

The new R-language package, *GCDkit.Mineral*, builds upon concepts introduced in Janoušek et al. (2006a) and its companion application *GCDkit* (Geochemical Data Toolkit), the latter providing tools for recalculation and plotting of bulk compositions of igneous and metamorphic rocks (Janoušek et al. 2006b; 2016). It uses a similar user interface, as well as many of the general routines for data input and output, data handling, statistics and graphics. For beginners all the functionality is accessible through menus, whilst more experienced R users may access the underlying functions and data via the command line.

Simplified program workflow

At the beginning of each session, raw (wt%) EPMA data in a matrix form are **imported** from the clipboard, plain text, CSV, Microsoft Excel XLS(X), Microsoft Access (MDB), or DBF files. The individual analyses are stored in rows; variables in columns may include a mixture of numeric data, textual meta-information (on mineral species, locality, etc.) and plotting properties (symbol, color and/or size) in essentially random order. Numeric data are automatically **recast to formulae** (apfu) using several methods (required number of O equivalents, number of atoms in the entire formula or part thereof, charge balance) with, or without, applying variable methods for Fe^{II}/Fe^{III} estimation. Default recalculation options for the individual mineral classes are stored in a plain-text file ('standard database') that may be edited by users without any prior experience with R. The calculated apfu are then **assigned to appropriate crystallographic sites,** and/or some **additional parameters**, such as Fe/Mg ratios, are computed. Furthermore, molar percentages of **end members** are obtained for minerals forming solid solutions. The individual analyses may be **classified** and **plotted** (as wt% concentrations or apfu/structurally allocated atoms) into binary and ternary plots, or their plates. The data can be **statistically treated** and remain available for any further calculations

within R, such as those used in thermobarometry. Finally, the results may be **exported** into a multitude of file formats (HTML, XLS(X), text files…) or **copied to clipboard**, and pasted e.g. into a spreadsheet or text editor.

'Under the hood' – technical implementation

The ideal solution for the development and distribution of mineralogical software is the Free and Open-Source Software (FOSS) model (Mader and Schenk 2017), utilizing one of the free, feature-rich, and platform-independent programming languages designed for scientific computation. This essentially rules out costly commercial packages such as Mathematica, MATLAB, S-Plus, or Statistica. However, the R language (Hornik 2021; R Core Team, 2021) provides a versatile and extensive environment for development of a geochemical recalculation, plotting and modelling software that can be far superior to dedicated programs and spreadsheets (Grunsky 2002; Janoušek et al. 2006b; Reimann et al. 2008; Janoušek et al. 2016). The R comes with generic tools for data import/export, recalculation (including matrix calculus), and descriptive/multivariate statistics, and produces publication-quality graphics. With its large and ever growing community, any R-based software has the potential of being extended fairly quickly by user additions.

In designing the *GCDkit.Mineral* R package, we make use of the concept of S4 classes (Chambers 1998). Thus, after loading, individual raw electron-probe micro-analyses are split into classes according to the mineral species to which they belong. This enables the recalculation and classification schemes to be defined as mutually independent, class-dependent calculations. The recalculation options for the given mineral class are stored externally in a small plain text file (*'mineral_db.r'*), which is read at startup (for details, see TABLE 1 and Electronic Supplementary Material, ESM 1).

The import and export of data in the CSV, XLS(X), MDB, DBF and HTML formats are facilitated by the *RODBC* and *R2HTML* packages (Ripley 2021 and Lecoutre 2003, respectively). Routines for effortless data management, i.e. grouping, searching, and generation of subsets, using regular expressions and Boolean logic are inherited from *GCDkit*. Diagrams are defined as templates for the internal graphical system 'Figaro' that provides a means to create and, if necessary, to later modify figure objects, for example changing the attributes of the plotting symbols, sizing, adding legend, or identification of individual data points.

Importantly, binary and/or ternary Figaro templates are used as a basis for classification. The classification schemes can be hierarchical to form decision trees. The classification algorithm looks for the name of the closed polygon within the graphical template (= diagram), into which the analysis falls according to its x–y coordinates. The outcome may be either a name of the mineral or a link to another diagram. In some cases, the classification is not done graphically, but (in part) using external functions.

The system can be effortlessly expanded by means of plugins, i.e. R code scripts stored in the eponymous subdirectory of the *GCDkit.Mineral* library. All these are automatically executed when the new data are loaded and can be made accessible via newly appended menus (Janoušek and Moyen 2014).

INTERNAL WORKINGS: A GUIDED TOUR THROUGH A DETAILED RECALCULATION SCHEME

This section explains the complete recalculation sequence. Calculations are invoked from menus and dialogs of the graphical interface unless the underlying functions are accessed directly in R.

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Loading data and assigning them to mineral classes (`minAssign`)

This function redistributes individual raw analyses of the input data matrix (`WR`) into a `min.data` list that contains named component(s) for each of the minerals present in the file, such as `min.data$garnet`. The mineral species (= class) is determined based on the column '**Mineral**' in the original file that can contain any of the full/abbreviated names defined in the standard database (including various formal or informal names in the given mineral group).

Each of these mineral objects (components in the `min.data` list) effectively represents a database with items named 'slots', such as `min.data$garnet@abbreviated` (TABLE 1). When the data set is loaded, slots with default recalculation options are copied from the standard database into each mineral object. Their possible combinations are illustrated in TABLE 2. Note that the properties (slots) not declared explicitly remain empty. After loading, the mineral data are split into a numeric part, i.e. the analyses themselves (slot `rough`) and textual information/plotting attributes (slot `labels`). The remaining slots are gradually filled as the calculation progresses.

Recalculation to atoms per formula unit (`minFormula`)

The function `minFormula` is a front-end to several specialized routines that calculate the apfu on the basis of a prescribed number of oxygen equivalents, atoms, or charges.

Fixed number of oxygen equivalents. The function `formulaFixedOxygens` recalculates mineral analyses to a given number of O equivalents as specified in the slot `oxygens`. Furthermore, the Fe^{II}/Fe^{III} ratio can be estimated by various methods as specified by the slot `iron` (see TABLE 1).

Alternatively, when both FeO and Fe_2O_3 have been determined, no Fe^{II}/Fe^{III} estimation is carried out and both oxides are recalculated as given. If necessary, the program can also

handle halogens, F and Cl (Deer et al. 2013). Here are some examples of appropriate entries in database (i.e. `mineral_db.r` file):

i. Recalculation to user-defined number of oxygens (4), no Fe^{II}/Fe^{III} estimation:

```
oxygens=4 # no @cations, @iron, @charges specified
```

ii. Recalculation to user-defined number of oxygens (12), estimation of Fe^{II}/Fe^{III} assuming a certain number of cations (8) in the whole formula (Droop 1987):

```
oxygens=12, cations=8, iron="Droop"
```

iii. Iterative recalculation to user-defined number of oxygens (12), estimation of Fe^{II}/Fe^{III} assuming a certain sum of cations (2) in a given site (Y), whose structure is described in the slot `"sites"`. In this example, the Y site is occupied by (part of) Al, Ti, Cr, Y, P and Fe^{III}:

```
oxygens=12, cations=2, cations.site="Y", iron="FixedCats",
sites=list(Z=c("Si","Al"), X=c("Mg","FeII","Ca","Mn"),
Y=c("Al","Ti","Cr","Y","P","FeIII"))
```

Fixed number of atoms per formula unit (or listed ones). The function `formulaFixedAtoms` recalculates chemical analyses to a given number of atoms. The sum is specified, for each mineral class, in the slot `atoms.sum`. The calculation is carried out for all atoms, or just those given in the slot `atoms.recalc.list` (if specified). Examples:

i. Recalculation to user-defined number of atoms (5) in the whole formula, without Fe^{II}/Fe^{III} estimation:

```
atoms.sum=5 # no @oxygens, @charges, @iron specified
```

ii. Recalculation to user-defined number (5) of selected atoms (Si + P), no Fe^{II}/Fe^{III} estimation:

```
atoms.sum=5, atoms.recalc.list=c("Si","P")
```

Fixed charges. The function `formulaFixedCharges` recalculates the mineral analyses using a charge-balance method. The number of desired charges is specified in the slot `charges`. Optionally, when slots `atoms.sum` and `atoms.recalc.list` are defined, Fe^{II}/Fe^{III} estimation can be carried out in an attempt to balance the formula precisely. For non-stoichiometric analyses, a warning message is displayed. On the other hand, when both FeO and Fe_2O_3 have been determined, no Fe^{II}/Fe^{III} estimation is carried out and both oxides are utilized as given. An example of recalculation to a certain number of charges (22) in the whole formula, without Fe^{II}/Fe^{III} estimation:

```
charges=22 # no @atoms.sum, @oxygens, @iron specified
```

and the same recalculation with Fe^{II}/Fe^{III} estimation:

```
charges=22,cations=7,atoms.recalc.list=c("Si","Al","FeIII","Mg","FeII")
```

Allocating apfu to crystallographic positions (`minAllocateAtoms`)

As the next step, this function allocates the computed apfu to crystallographic sites of the given mineral(s). The sites are filled by each of the atoms in the order specified, from left to right, in the slot `sites`. If some of the atoms may be present in two sites, the slot `site.sums` must give the required sum for the first of them. As soon as the first site is filled (the sum in `site.sums` is reached), any excess of the given element is passed to the next position available. In the following example:

```
sites=list(Z=c("Si","Al"),X=c("Mg","Fe"),Y=c("Ti","Al")),
site.sums=c(6,NA,NA)
```

the site 'Z' is filled with all Si and part of Al (6 – Si). Any excess Al will be transferred to the site 'Y'. In other words: `Al_Z = 6 - Si_Z; Al_Y = Al - Al_Z`.

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In this case, no `site.sums` have to be defined for sites 'X' and 'Y', hence the `NA` value (`NA` standing in R for 'not available'). If desired, a special symbol for vacancy (`Vc`) can be introduced if the site is to be filled up by vacancies to the specified sum. The crystallochemical formulae can be visualized using the function `HTMLformula`, attached to the menu *Calculations*|*Export structural formulae to HTML*.

Calculating additional parameters (`minValues`)

At this point, extra values may be calculated either by an external R script or as specified by formulae stored in the standard database (in the slots `values.formulae` and `values.names`). An example:

```
values.formulae=c("Ca/(Ca+Mg+FeII+Mn)", "FeII/Mg", "Al_Z/Al_Y"),
values.names=c("XCa","Fe2+/Mg","AlIV/AlVI")
```

The `values.formulae` can refer to valid atom names (from the slot `recalc`), and/or the names of the atoms allocated to the crystallographic sites (stored in the slot `formula`), as does the third item above, referring to Al atoms in positions 'Z' and 'Y'.

Obtaining mol% of endmembers (`minEndMembers`)

The molar proportions of end-members can be calculated by an external R script or by formulae given in the database (slots `end.member.names` and `end.member.formulae`).

Thus, for feldspars (simplified):

```
end.member.formulae=c("Na/(Na+Ca+K)","Ca/(Na+Ca+K)","K/(Na+Ca+K)"),
end.member.names=c("Ab","An","Or")
```

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Note that the formulae may again refer to valid atom names and/or names of the atoms allocated to the individual crystallographic sites and/or special parameters calculated at the previous step. See the following simplified example:

```
values.formulae=c("FeII/(Ca+Mg+FeII+Mn)","Mg/(Ca+Mg+FeII+Mn)",
    "Mn/(Ca+Mg+FeII+Mn)"), values.names=c("XFe","XMg","XMn"),
end.member.formulae=c("XMg","XFe","XMn","FeIII/2"),
end.member.names=c("Prp","Alm","Sps","Adr")
```

FOR ADVANCED USERS: USING GCDKIT.MINERAL IN DIRECT OR BATCH MODE

GCDkit.Mineral contains several built-in training datasets, derived from the third edition of the monograph by Deer et al. (2013). These are invoked by command `sampleDataset(mineral)`. Available now are the following datasets: `alumosilicates, amphibole, apatite, feldspars, garnet, micas, olivine, pyroxene.`

Apart from the menus, the *GCDkit.Mineral* code can be called in direct or batch mode. In both cases, the `minMain` front-end function can invoke on-demand recalculation of chemical analyses by specifying the mineral name and an (optional) list of recalculation options as arguments. Note that all obsolete options are cleared automatically, before the newly desired ones are set. Examples of custom recalculations:

```
sampleDataset("garnet")
minMain("garnet") # default options (from the standard database)
minMain("garnet",list(oxygens=12))
minMain("garnet",list(oxygens=12,cations=8,iron="Droop"))
minMain("garnet",list(oxygens=12,cations=2,cations.site="Y",
    iron="FixedCats"))
minMain("garnet",list(atoms.sum=8))
```

```
minMain("garnet",list(atoms.sum=8,values.formulae="Al_Z/Al_Y",
    values.names="Al ratio"))
sampleDataset("amphibole ")
minMain("amphibole",list(oxygens=23,iron="13eCNK"))
sampleDataset("pyroxene")
minMain("clinopyroxene",list(oxygens=6,iron="PxPapike"))
```

Note that the crystallographic site allocations, calculations of extra values and end-members, may not be compatible with the chosen user-defined recalculation method. For example, if `site.sums` of `c(2,2,NA)` are defined in the standard database for recalculation to 8 O equivalents, they need to be doubled if recalculating to 16 O:

```
minMain("feldspar",list(oxygens=16,site.sums=c(4,4,NA)))
```

DISCUSSION

The *GCDkit.Mineral* package provides a versatile, free, open, and platform-independent alternative to the existing software for recalculation and plotting of mineral chemical analyses, nowadays obtained chiefly by microbeam techniques. Its modular nature allows for easy introduction of new recalculation schemes for missing mineral classes, or tailoring the existing ones. Lastly, *GCDkit.Mineral* offers a gateway for petrologists and mineralogists to the wealth of plotting and statistical functions embedded in the R language. We review advantages and shortcomings of our software compared to the existing packages, describe the scope of its applications in respect to the needs of various user groups and outline possible future developments.

Comparison with existing software

Based on the scope, the existing software for recalculation of mineral compositions may be subdivided into two types.[1]

'Universal' programs applicable to several mineral groups. Only a handful of authors have attempted to develop a universal recalculation package that may deal with a larger number of mineral species/groups. On recent (32- and 64-bit) Windows systems, these have been CALCMIN (Brandelik 2009) and MINCALC (Bernhardt 2010). The more versatile, platform-independent tools invariably use universal computing environments, such as Mathematica® (PET: Petrological Elementary Tools – Dachs 1998; 2004), or MATLAB® (MINERAL – De Angelis and Neill 2012; MinPlot – Walters 2022). XMapTools (Lanari et al. 2014; 2019) have special standing, offering a feature-rich environment for treatment of mineral data, including plotting and mineral formula calculations. Even though MATLAB-based, this software comes with a runtime module and thus is freely available both on Windows and Mac. A similar future is apparently also planned for MinPlot (Walters 2022).

Software specialized to a single mineral group. Numerous packages have been designed for recalculations, classification, and geothermobarometry of individual mineral groups, mostly as MS Excel spreadsheets or standalone Visual Basic programs (TABLE 3). These often offer countless features and calculation options, and in that respect are inevitably superior to any universal tools.

Disadvantages of existing software. *Spreadsheets* are complex and prone to errors. There is limited protection of the primary data as they are mixed together with the algorithms

[1] The following list does not aim to be exhaustive; especially for the mineral-specific dedicated programs, this is meant to provide some examples, admittedly with a strong MS Windows bias.

and calculated results. The quality of the graphical output lags behind the standards required for scientific publication.

The *dedicated programs* are difficult or impossible to alter. Most of them are available only on a single platform (typically MS Windows), have complicated data input, and often lack graphics – some relying on external proprietary software to produce it (e.g., *Grapher* for numerous specialized programs by Yavuz and coworkers). Many have been designed for now obsolete operating systems, most notably 16-bit-based ones (DOS, Windows 3.x, Windows 95/98/ME).

The *platform-independent tools* commonly use costly computing environments (Mathematica or MATLAB), which hinders their uptake in the scientific community, especially in economically challenged countries. In addition, some of them (e.g., PET, MinPlot) are not menu-driven, and a command-line interface may represent a psychological barrier to ordinary users. XMapTools have their focus mainly on spatial data treatment (chemical maps); their mineral recalculation functions are directed mainly to geobarometry and, eventually, petrochronologic applications.

Advantages of *GCDkit.Mineral.* Our package can import essentially free-form data in a variety of file formats or simply by reading the clipboard. The data, both original and recalculated, can be plotted onto (near) publication-ready diagrams (binary and ternary plots, histograms, boxplots, etc.). Most of them can be retouched and all saved into a number of vector-based (PostScript, PDF and WMF) and bitmap-based (e.g., PNG, TIF and JPG) file formats, ready to be imported into a professional graphical, presentation or desktop-publishing software. Binary and ternary plots can be combined with simple R scripts to create hierarchical classification schemes. The data are ready for further treatment, both by *GCDkit.Mineral* or R itself, including descriptive statistics and multivariate methods, e.g., clustering and principal components. The bulk compositions of the host rocks can also be

integrated, as required by some thermobarometers. The whole system is platform-independent, open, customizable, and expandable.

Field of application. The *GCDkit.Mineral* package caters to several user groups.

For the novice R user, it provides a graphical interface that is accessible regardless of little to no knowledge of computer coding, retaining much logic and functionality familiar to seasoned *GCDkit* users. For petrologists or igneous/metamorphic geochemists, it comes with pre-defined recalculation schemes for a range of common rock-forming and accessory minerals appropriate for most standard applications.

Our package also serves experienced mineralogists. Although many of the suggested schemes are admittedly not universally applicable or accepted, the standard database of recalculation options stored in the plain text file is easy to alter without prior R programming skills. Furthermore, it sets an example for editing existing recalculation schemes, or even introducing new mineral classes.

Colleagues with R knowledge can invoke *GCDkit.Mineral* in direct mode, or, furthermore, can recall the recalculated data for further plotting and statistical treatment within the R. Writing and running own R scripts (batch mode) is advantageous, especially when large datasets are to be recalculated, or the same approach is to be applied routinely to multiple files.

Arguably the most useful is the possibility of invoking *GCDkit.Mineral* from Python-driven interactive notebooks (Shen 2014), the most popular currently being the project *Jupyter* (*http://jupyter.org*). They combine formatted explanatory text with static images and mathematic formulae, computer code (including R), and its textual and graphical output. The

code can be modified and executed directly in the web browser; the kernel connects the notebook to the R interpreter running seamlessly in the background. Static Jupyter notebooks can even be viewed without installing Python, R, *GCDkit.Mineral* and *Jupyter*, e.g., by simply using the online *nbviewer* (*http://nbviewer.jupyter.org*).

Again, Python-driven interactive notebooks are good for mutating data sets and repeated tasks, as well as for experimenting with various approaches. In addition, they represent an ultimate teaching tool and provide an efficient remedy to the 'reproducibility crisis' in that they are ideal for documenting, sharing and reproducing research results. An example of a *Jupyter* session with *GCDkit.Mineral* is given in ESM 2.

Known limitations. The current version is intended for processing of EPMA data, possibly with supplementary FeO and Fe_2O_3 analyzes obtained by an alternative method. So far, it cannot handle other elements with multiple valencies (such as Mn) and no H_2O determinations are taken into account. At the moment, OH^- is simply estimated by difference in the OH site (if F and Cl are known), and such an approach is clearly not satisfactory for some mineral compositions, e.g. for oxyamphiboles. Future releases of *GCDkit.Mineral* should allow import and treatment of supplementary trace-element data, acquired by laser-ablation inductively-coupled mass-spectrometry (LA ICP-MS) or ion probe. It will also implement the graphical tools necessary for their interpretation, such as spiderplots.

The palette of implemented classification schemes and pre-defined graph templates for individual minerals remains limited. Also, the possibility of switching/overplotting multiple datasets, available in *GCDkit*, is to be introduced in some future release. On Linux and Mac, the data can be currently imported (exported) solely from (to) text files (TXT, CSV), clipboard or DBF files; also some other functionality (like command history or interactive of editing of plates of several graphs) cannot be implemented.

IMPLICATIONS

The newly designed R package provides a platform-independent, lucid, and flexible computing environment for treatment of mineral composition data. There is no copyright protection that would hinder modifications (FOSS, Free and Open-Source Software) and the whole package has an open architecture.

Even for novice R users, *GCDkit.Mineral* is effortlessly customizable and expandable. As the recalculation options are stored in an easy-to-understand, plain text file, they can be tweaked, and brand new mineral classes (or subclasses) introduced. For users with R programming knowledge, the system is expandable by external plugins for, *inter alia,* further computations and plotting of recalculated data, statistics, or geobarometry. The workflow can be automated by scripting or using Python-driven interactive notebooks. This approach is advantageous for working with large and/or mutating datasets, has great teaching potential and facilitates reproducibility of research.

Therefore, the *GCDkit.Mineral* provides not only a workbench for daily ordinary recalculations and plotting in petrology and mineralogy, but also a flexible platform for community-driven development of new tools dealing with mineral compositional data. These may take the form of plugins, or even full-blown packages dependent on *GCDkit.Mineral*.

AVAILABILITY

The current version of the *GCDkit.Mineral* package, together with the appropriate version of R, can be downloaded from *http://mineral.gcdkit.org*. The package has been developed on Windows 10 but should run on Windows 7 and above. With some limitations – mainly regarding the file formats available for import/export – it can be installed also on Mac OS X (release 10.6 and above) and various distributions of Linux (Mint, Debian, RedHat, SUSE, Ubuntu).

Instructions for installation of the described Windows *GCDkit.Mineral* 1.0 version for R 4.1.3 are given in ESM 3. The electronic supplement also contains information about the selected system variables (ESM 4) and useful internal functions (ESM 5).

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587

FIGURE CAPTIONS

FIGURE 1 An example of the *GCDkit.Mineral* session with Tcl/Tk menus on Mac (top), and an example of Jupyter notebook (bottom).

FIGURE 2 Tentative scheme for clinopyroxene recalculations, plotting and classification using the *GCDkit.Mineral*. Note that the database entry is strongly simplified to illustrate the general principles.

TABLE CAPTIONS

TABLE 1. Standard database structure (the main database slots) for each mineral object

TABLE 2. Available formula recalculation options

TABLE 3. Overview of recent Windows software for recalculation of selected mineral groups

ELECTRONIC SUPPLEMENTAL MATERIAL

ESM 1 Recalculation schemes implemented for the individual mineral classes

ESM 2 Example of interactive mineral calculations and plotting in a Jupyter notebook

ESM 3 Instructions for installation on MS Windows, Mac and Linux

ESM 4 Selected system variables

ESM 5 Useful functions

TABLE 1. Standard database structure (the main database slots) for each mineral object

Recalculation options

Slot	Explanation
`full` `abbreviated`	All possible full names/abbreviations recognized as the given mineral class. The latter include the standard ones from Kretz (1983), Whitney & Evans (2010) and Warr (2021), as well as those used by other software packages, e.g. MinPet (Richard 1995), Thermocalc (Holland and Powell 1998) or PET (Dachs 1998; 2004).
`oxygens`	Number of O equivalents the formula should be recalculated to.
`charges`	Number of charges to which the formula should be recalculated; optionally, Fe^{II}/Fe^{III} estimation can be carried out in an attempt to balance the formula precisely.
`atoms.sum`	Number of atoms in the formula unit (recalculations to a desired number of atoms – i.e., neither `oxygens` nor `charges` are given).
`atoms.recalc.list`	Atoms that are to be summed (for formula recalculation to a desired sum of specific atoms).
`cations`	Number of cations when Fe^{II}/Fe^{III} is to be estimated by the methods `Droop` (referring to the total sum of cations) or `FixedCats` (giving the sum of the site specified by `'cations.site'`).
`cations.site`	Name of the site that should be summed by iterative iron estimation (if `iron = "FixedCats"`).
`iron`	Fe^{II}/Fe^{III} estimation method, implemented are `'Droop'` and `'FixedCats'`, `'allFeII'` and `'allFeIII'`. For amphiboles can be used also `'8Si'`, `'16CAT'`, `'15eNK'`, `'15eK'`, `'13eCNK'`, `'8SiAl'`, `'10sumFeIII'`, and `'avg'`, for pyroxenes also `'PxPapike'`.
`atom.names`	Names of all possible atom names to be returned by formula recalculation (though not all need to be present in the current data file).
`sites`	List, whose each component contains names of atoms that should be allocated to the given crystallographic site.
`site.sums`	Sums of individual sites, or *NA* when not needed/known.
`values. formulae`	Formulae for calculation of additional parameters (or the name of an external R script).
`values.names`	Their names.
`end.member.formulae`	Formulae for calculation of end members (or a name of an external R script).
`end.member.names`	Their names.

Mineral data (original and recalculated)

Slot	Explanation
`rough`	Original analyzes (wt%) as imported from the data file, but there may be some additions calculated by the system based on mineral stoichiometry (indicated by asterisks), such as H_2O* or Fe_2O_3* or FeO*.
`labels`	All at least partly textual information on individual analyses from the file plus plotting attributes (plotting symbols, their colors, sizes).
`recalc`	Analyses recalculated to apfu.
`formula`	Atoms per formula unit allocated to crystallographic sites.
`values`	Computed extra parameters.
`end.members`	Molar proportions of end members in a solid solution.

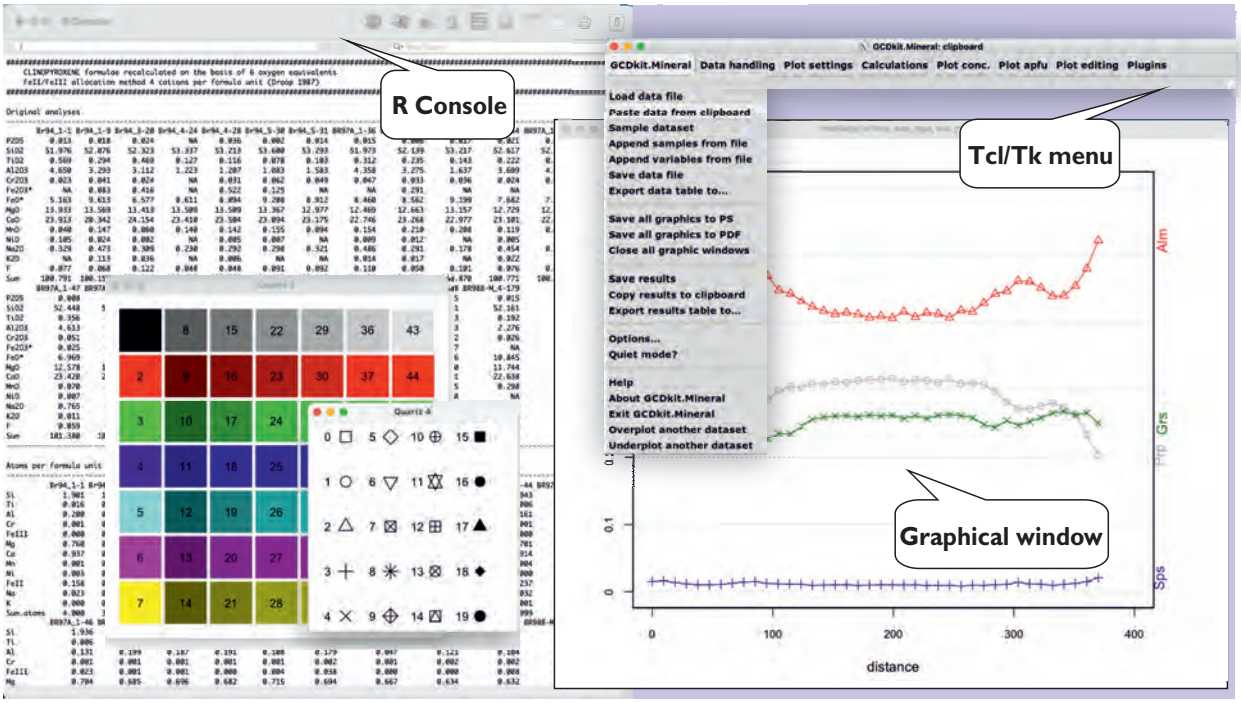
TABLE 2. Available formula recalculation options

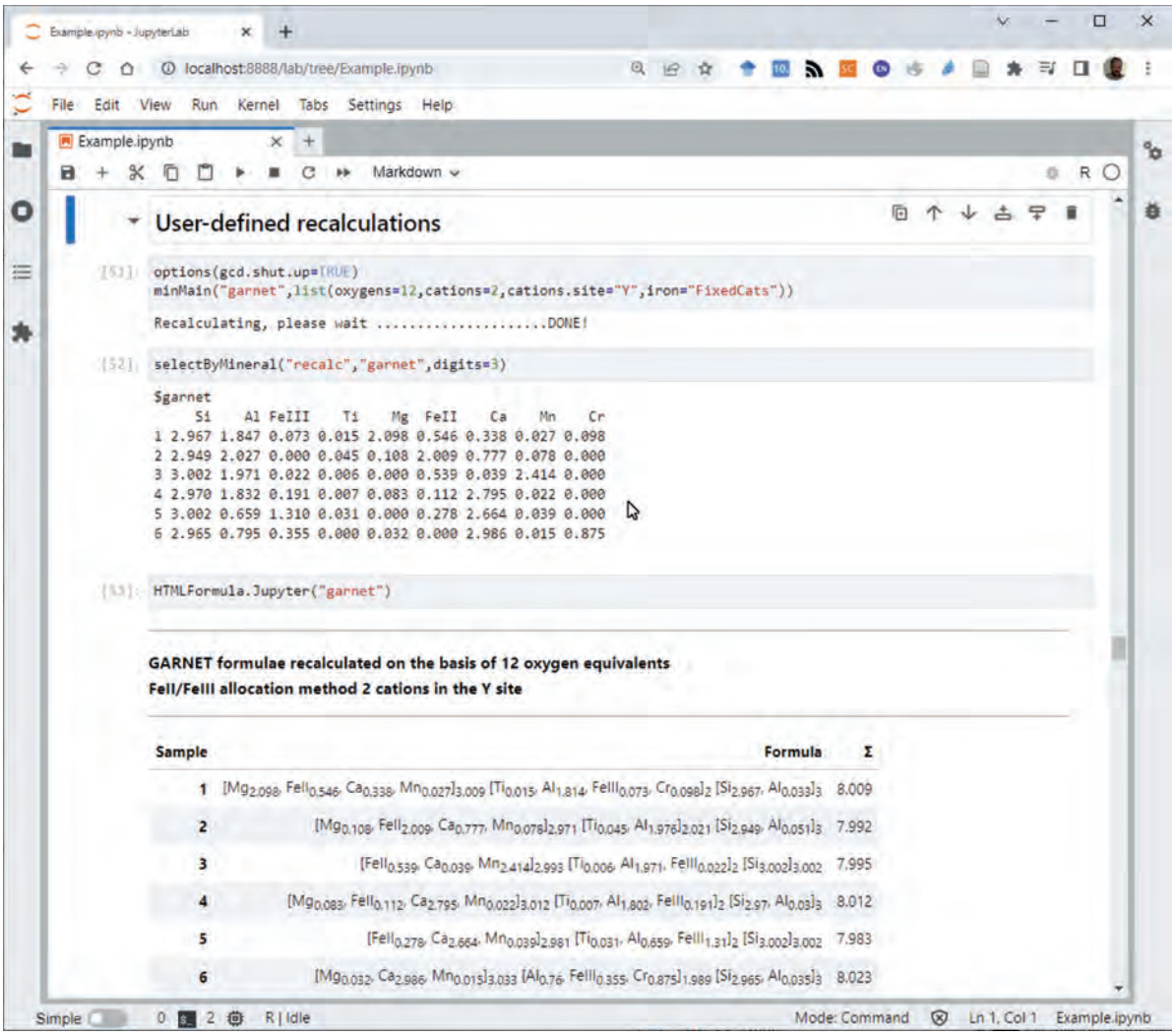
Slot/Recalculation type	`oxygens`	`charges`	`atoms.sum`	`atoms.recalc.list`	`cations`	`cations.site`	`iron`
No Fe^{II}/Fe^{III} estimation							
Given number of cations in entire formula			●				
Given number of selected atoms (here Si + P)			●	`c("Si","P")`			
Given number of O equivalents	●						
Given number of charges		●					
With Fe^{II}/Fe^{III} estimation							
Given number of O equivalents, Fe^{II}/Fe^{III} estimation assuming total number of cations in the whole formula	●				●		`"Droop"`
Given number of O equivalents, Fe^{II}/Fe^{III} estimation assuming a certain number of cations in the specified site (here Y)	●				●	"Y"	`"FixedCats"`
Given number of charges, Fe^{II}/Fe^{III} estimation to balance the formula		●		●	●		

● – number to be set (other slots remain empty

TABLE 3. Overview of recent Windows software for recalculation of selected mineral groups

Mineral group	Name	Reference	Programming environment
Amphiboles	*PROBE-AMPH*	(Tindle and Webb 1994)	MS Excel spreadsheet
	AMPH-CLASS	(Esawi 2004)	MS Excel spreadsheet
	WinAmphcal	(Yavuz 2007)	Visual Basic
	AMPH2012	(Locock 2014)	MS Excel spreadsheet
	WinAmptab	(Yavuz and Döner 2017)	Visual Basic
	AMFORM	(Ridolfi et al. 2018)	MS Excel spreadsheet
Garnets	*'Supporting Information A'*	(Locock 2008)	MS Excel spreadsheet
	garnet.R	(Arai 2010)	R language script
	'Appendix 4'	(Grew et al. 2013)	MS Excel spreadsheet
	WinGrt	(Yavuz and Yildirim 2020)	Visual Basic
Pyroxenes	*PYROX*	(Yavuz 2001)	Visual Basic
	PX-NOM	(Sturm 2002)	MS Excel spreadsheet
	WinPyrox	(Yavuz 2013)	Visual Basic
	WinPLtb	(Yavuz and Yildirim 2018b)	Visual Basic
Spinels	*WinSpingc*	(Yavuz and Yavuz 2023)	Visual Basic
Tourmalines	*WinClastour*	(Yavuz et al. 2006)	Visual Basic
	WinTcac	(Yavuz et al. 2014)	Visual Basic
Feldspars	*WinFeldth*	(Yavuz and Yavuz 2022)	Visual Basic
Epidotes	*WinEpclas*	(Yavuz and Yildirim 2018a)	Visual Basic
Micas	*Mica+*	(Yavuz 2003a; 2003b)	Visual Basic
Chlorites	*WinCcac*	(Yavuz et al. 2015)	Visual Basic



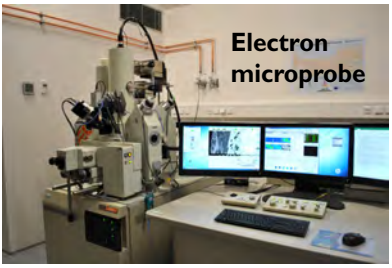


Janoušek et al., Fig. 1
Double column width

Chemistry
Formula
Classification
Crystallization T (°C)
Depth (pressure)...

```
################################################################################
#                                CLINOPYROXENE                                 #
#                            M2[1]M1[1]T[2]O[6]                                #
################################################################################
setClass("clinopyroxene",representation(),contains="mineral",
    prototype(
        abbreviated=c("Px","Cpx","Aeg","Ae","Aug","Di","Hd","Jd"),
        full=c("clinopyroxene","Ca clinopyroxene","aegirine",
            "augite","clinoenstatite","clinoferrosilite",
            "diopside","hedenbergite","jadeite"),
        oxygens=6, cations=4,
        iron="Droop",
        atom.names=c("Si","Al","FeIII","FeII",
            "Ti","Cr","V","Zr","Zn","Ni","Co","Mg","Mn",
            "Li","Ca","Na","K"),
        sites=list(T=(c("Si","Al","FeIII")),
            M1=c("Al","FeIII","Ti","Cr","V","Zr","Ni","Co","Mg","FeII","Mn"),
            M2=c("Mg","FeII","Mn","Li","Ca","Na","K")),
        site.sums=c(2,1,NA),
        values.formulae="clinopyroxene.r",
        values.names=c("FeIII/Fetot","XMg","AlIV/AlVI","AlIV","AlVI","aDi"),
        end.member.formulae="clinopyroxene.end.r",
        end.member.names=c("Jd","CaTs","CaTi","CrCaTs","DiHd","EnFs")
))
```

S4 Class
"clinopyroxene"



All recalculation options for each mineral class
(stored in an external plain text file)

Spot chemical analyses
(clipboard, TXT, CSV,
XLS(X), MDB, DBF...)

Assigning the mineral classes
`minAssign()`

Recalculation to apfu
(fixed O eq., cations, charges)
`minFormula()`

Allocating apfu to
crystallochemic sites
`minAllocateAtoms()`

Additional parameters
`minValues()`

Molar % of end members
`minEndmembers()`

Classification
`classify()`,
`minClassifyPlot()`

etc. etc.

Statistics
(descriptive, cluster,
PCA, LDA...)

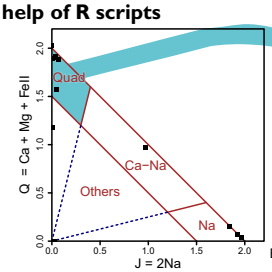
Recalculated data
(clipboard, TXT, CSV,
XLS(X), HTML, DBF...)

Graphics
(PDF, PS, EPS, WMF,
PNG, TIFF, JPG...)

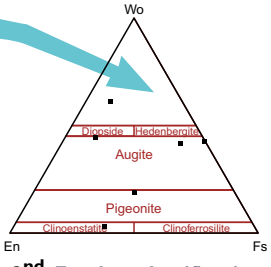
GCDkit.Mineral

- **FIGARO** = a set of graphical utilities implemented in ***GCDkit-Mineral***
- **Tools to create figure objects, containing both data and methods to make subsequent changes to plot**
- **Editing before committing to hardcopy (e.g., changing colors and scale of plotting symbols, zooming, interactive identification of data points etc.)**
- **Closed polygons defined on binary and ternary plots provide a basis for classification**

- **CLASSIFICATION** = **Pre-defined hierarchical sequence of steps, for each class based on binary and/or ternary Figaro templates, with, or without, help of R scripts**



1st Preliminary classification in the Q–J diagram...



2nd: Further classification applicable to "Quad" field...

Janoušek et al., Fig. 2
Double column width