

MINCALC-V5, A SOFTWARE TOOL FOR MINERAL ANALYSES DATA PROCESSING

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In many laboratories mineral analyses are carried out by means of an electron microprobe or a scanning electron microscope with an attached energy-dispersive spectrometer. Besides tabular or graphical presentation of the analyses, formula recalculation is needed for a complete analyses evaluation. This may include the calculation of unmeasured elements such as Li, B, O and H or the separation of Fe into Fe²⁺ and Fe³⁺. In addition simple long term storage and retrieval must be guaranteed. In order to perform the requested computations special programs for each mineral or EXCEL are used. Only few general programs exist for this application. Most of them, however, are not really flexible as they use procedures, which are difficult or not at all adoptable by the user to his specific problems.

MINCALC-V5 combines a) storage and retrieval of analyses data, b) simple and versatile analyses selection, c) flexible output, d) formula recalculation, which may be programmed by the user, e) simple plotting of all measured and computed variables.

The general structure of MINCALC-V5 is depicted in Fig. 1. In a very first step analyses files, which were generated by the various measuring instruments have to be converted to a special MINCALC-V5 file. Manual input is also possible. Besides all other needed analyses information, date and user name are stored.

When reading a MINCALC-V5 file, an array is filled with all analyses. It contains only the measured element concentrations. In that moment all analyses are declared to be selected and the "selected analyses array" is filled again with elements but also with atomic proportions (ATP) and upon request with oxides of the measured elements using default valences. When anions like fluorine or chlorine were measured, a correction of the calculated oxygen is done automatically. All values in the aforementioned array are ready for output and plot as well as for basic computations like normalisation of the ATPs using a selectable variable, rearrangement for one variable or calculation of basic statistics (minimum, maximum, mean etc.).

Normally raw analyses files contain data of various minerals of different samples as well as bad analyses. Therefore diverse possibilities of analyses selection are available: single analysis with a mouse click, application of a sophisticated value filter, rearrangement using one variable, rearrangement using one analysis as pattern for a similarity investigation of all analyses, even plots may be used to select analyses. Once analyses are selected they may be combined with a key. That means, when e.g. a certain mineral is selected, the mineral key is used to name it. Furthermore a sample key exists and a key for free use. Bad analyses can be blocked without deleting them in a similar way. Keys are stored together with the analyses and may be applied later. Thus it is e.g. possible to rapidly find the analyses of a certain mineral of a certain sample. Only selected analyses are available in the "selected analyses array" for further actions like output, plot or recalculation.

At the moment following plot possibilities are implemented: histogram, line-scan, X-Y-Plot and triangular plot. When the mouse pointer is moved on an analysis symbol, the number of the related analysis is indicated and all other variables can be displayed upon request. Plots may be stored in a file or copied to the clipboard for further use.

For the generation of an output list all currently available variables are displayed. A simple click on a variable moves it to the cursor position in the list. Thus, a user-defined output sequence can easily be established or modified. The formatted data may just be displayed but also stored in a named file. It is also possible to store the data in a file, which can be imported to EXCEL

The most important part of MINCALC-V5 is the “programmed recalculation” to obtain structural mineral formulae. A simple language has been developed as well as a simple graphical programming environment to write calculation procedures. The language comprises routines for calculation (like: SUM(list), CHARGE(list), FILL, AGE, STATISTICS etc.) and statements for program control (like ITER, END_ITER, EXIT_ITER, IF, ENDIF, DISPLAY etc.) Tested recalculation programs may be stored for later use including the appropriate output list. They are easy to understand and to modify by further users.

MINCALC-V5 has access to a list of nearly all currently known minerals and their formulae. With a special routine their wt% compositions may be computed helping to assess analyses of hitherto unidentified minerals.

At the Ruhr-University MINCALC-V5 has been tested for about two years and it is used at moment by several external testers.

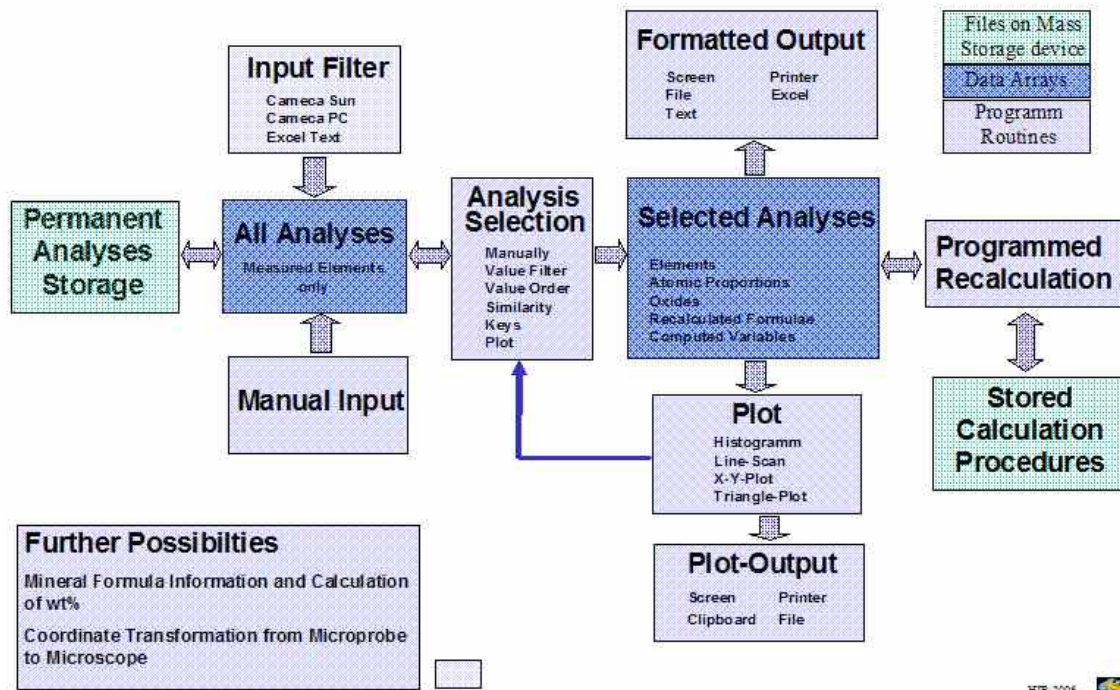


Fig 1: General structure of MINCALC-V5