"PETROGRAPH": A NEW SOFTWARE FOR THE ANALYSIS AND PRESENTATION OF GEOCHEMICAL DATA

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Evaluation, presentation and interpretation of geochemical data are fundamental operations in igneous petrology. Several software are available at present to perform most of operations needed to generate petrological plots and classification diagrams as well as to calculate geochemical models. Most of these software run on MS-DOS or MS-Windows platforms but in most cases they have severe limitations such as, for example, the inability to import MS-Excel worksheets or they lack of important classification diagrams that generally are time consuming to perform utilising general purpose plotting packages. In addition, some important petrological models cannot be readily performed and difficulties arise in the management of plots for presentation or publication purposes. The software "Petrograph" is an answer to all these difficulties and it is specifically intended to bridge the gap between manipulation, analysis and presentation of geochemical data in igneous petrology.

The source code of "Petrograph" is written in MS-Visual Basic 6.0 and, as such, the software runs on Windows 98/2000/XP platforms. The software is able to import a variety of pre-formatted data files such as ASCII and MS-Excel worksheets. Data can be visualized using several types of plots including binary and triangular plots, and spider diagrams; in addition, a large number of classification and discriminating diagrams are ready to use with a simple click of mouse. Various options are present in each type of diagram in order to help the users to develop publication quality plots that can be easily exported as MS-metafiles (.wmf) into any other graphical software using both the MS-Windows clipboard or by saving directly the file onto the hard disk and than re-importing.
Data can be treated in a variety of ways including mathematical operations and determination of the most used geochemical parameters and indexes. Mathematical operations include sum, subtraction, multiplication, division, exponent, and square root. The principal geochemical parameters and indexes which can be determined are: CIPW norm, Larsen Index, Solidification Index, Total Iron and Fe/Mg Ratio; weight per cent values can be converted in molar values and REE parameters can be calculated. Large number of geochemical models can be calculated and plotted: Batch Melting (modal and not), Fractional Melting, Continuous Melting, Zone Refining, Fractional Crystallization, Equilibrium Crystallization, in Situ Crystallization, Mixing, O’Hara’s RFT and RFT(A), DePaolo’s AFC. The models are performed using trace elements and, when possible, isotopes.

"Petrograph" graphical interface has been specifically designed to be user friendly and to allow even users with little knowledge of computer techniques to manage and plot geochemical data. Thanks to its intuitive interface "Petrograph" can be utilised for research purposes as well as for teaching and training activity.