WinPyrox: A Windows program for pyroxene calculation classification and thermobarometry[†]

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ABSTRACT

A Microsoft Visual Basic program, called WinPyrox, has been developed to calculate structural formulas of both wet-chemical and microprobe-derived pyroxene analyses. Based on the standard International Mineralogical Association (IMA-88) nomenclature scheme, WinPyrox primarily calculates and classifies pyroxene groups and then determines a specific pyroxene name with its possible modifiers. It is developed to predict cation site-allocations at the different structural positions, including T, M1, and M2 sites, as well as to estimate end-members, molar fractions, end-member activities, components and activities, and single-clinopyroxene and two-pyroxene thermobarometers. The program allows the user to edit and load Microsoft Excel files to calculate electron-microprobe pyroxene analyses for different ferric iron estimation methods and normalization schemes. This software generates and stores all the calculated results in the output of a Microsoft Excel file, which can be displayed and processed by any other software for verification, general data manipulation, and graphing purposes. The compiled program code is distributed as a self-extracting setup file, including a help file, test data files, and related graphic files, which are designed to produce a high-quality printout from the Golden Software's Grapher software. The self-extracting setup file, which is approximately 12 Mb, may be downloaded from http://code.google.com/p/winpyrox/ or can be obtained from author on request.

Keywords: International Mineralogical Association (IMA), pyroxene, classification, modifier, end-member, activity, thermobarometer, normalization, software