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PetThermoTools: a fast, flexible and accessible Python3 package for performing thermodynamic calculations for petrological research and teaching

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We present PetThermoTools- an open-source Python3 tool for performing thermodynamic simulations of mantle and magmatic processes. Thermodynamic modeling forms a central component to many research projects in igneous petrology. However, few studies utilize the full potential of these methods due to the steep learning curve associated with existing code or text-based interfaces (e.g., ENKI/Thermoengine, alphaMELTS, Theriak-Domino) and the limited model flexibility provided by spreadsheet and GUI based packages (e.g., MELTS for Excel). We designed PetThermoTools to bridge this divide, providing logical, easy to-use functions with well-documented examples for novice users, while retaining the potential for customization and model automation desired by more experienced users. PetThermoTools also provides the opportunity to directly compare multiple different thermodynamic models and approaches, by integrating with both the alphaMELTS and MAGEMin packages. Furthermore, PetThermoTools model outputs seamlessly integrate with other Python-based packages created for petrological research (e.g., PySulfSat, Thermobar), and provide speed and stability advantages over existing free MELTS-based software owing to the use of parallel processing routines. We will present a number of example calculations, demonstrating how easy the code is to interact with, and how the inbuilt plotting functions can be used for exploring outputs (e.g., Harker diagrams, phase abundance diagrams, plotting ternary diagrams of outputs etc.). We will also discuss how PetThermoTools can be used as part of Petrology and Volcanology classes to help students to develop an intuition for how magmatic systems work (e.g., exploring how changing P-T-X changes the liquidus phase, how H_2O and fO_2 control the development of calc alkaline and tholeiitic trends, and what happens to volatiles during ascent from the mantle, differentiation and magma decompression).

Extensive documentation is available on ReadTheDocs (https://petthermotools.readthedocs.io/en/latest/), with narrated YouTube worked examples and recorded workshops on YouTube (https://www.youtube.com/@PetThermoTools). We are actively continuing to expand the PetThermoTools functionality, including co-developed engines for handling trace element partitioning and stable isotope fractionation.

References