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Pytheriak – A user-friendly python wrapper for Theriak

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Predicting the mineral-fluid assemblage, modes, and compositions in a rock at a pressure and temperature of interest is crucial for all studies requiring robust petrological constraints. Equilibrium thermodynamics and Gibbs energy minimisation (GEM) lay the theoretical groundwork to approach this problem. Several open-source programs implementing an algorithm for GEM in complex geochemical systems are available (e.g., Theriak-Domino: De Capitani and Brown, 1987; MAGEMin: Riel et al., 2022). However, the application of those programs is limited to routines and scenarios implemented by the original authors.

Here we present pytheriak, an easy-to-use package to conduct Theriak-GEM in Python programs. Pytheriak can be used in any chemical and physical models that require on-the-fly GEM. Thermodynamic state variables of the minimised system are saved in a *pytheriak.Rock*-object allowing the user to extract specific information for their scientific problem. Users can access several properties including: G_{system}, volume proportions, mineral or fluid composition.

The pytheriak package offers user-friendly tools to run a large number of GEMs, visualise minimisation results, adapt complex modelling strategies, and couple thermodynamics with physical models. Example applications are (1) plotting phase relations in a metamorphic rock along a pressure – temperature path; (2) fractionating phases (minerals or melts) to model a dynamically evolving reactive bulk composition; and (3) exploring phase compositional trends within and across thermodynamic databases.

Pytheriak is open-source and available on github (github.com/Theriak-Domino/pytheriak). The package can be installed with *pip* from the Python Package Index.

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