pyrolite: Python for Geochemistry

A set of tools for making the most of your geochemical data.

Morgan Williams1*, Louise Schoneveld2, Yajing Mao3, Jens Klump3, Hayden Dalton3, Adam Bath1 and Steve Barnes1

1: CSIRO Mineral Resources
2: Institute of Geology and Geophysics, Chinese Academy of Geosciences
3: School of Earth Sciences, University of Melbourne

* Authors listed in reverse alphabetical order.

Free and open source tools for geochemical transformation and visualisation
Community-driven project and repository for reference compositions and models
Beginner friendly and well documented

Open Science, Python & Open Source

The Open Science movement calls for more transparent, cooperative and collaborative scientific research. This encompasses many aspects from open data to open publishing, but requires that the tools and software we use to conduct research are also accessible and transparent. The geochemistry community is increasingly adopting digital approaches to research, but there are few open software options. Using open software as part of this shift can ensure that our research and tools used to achieve it are accessible to all.

The scientific Python ecosystem provides a ‘batteries-included’ set of libraries which users can leverage to rapidly prototype and develop data analysis, modelling and visualisation solutions. Using a programmatic approach for data analysis and documentation enables this aspect of research to be effectively reproduced and versioned, and greatly increases transparency.

pyrolite

pyrolite is an open-source python package built to facilitate data-driven understanding of geological processes using multivariate geochemical data. It has been built with the aim of contributing to more robust and efficient geochemical research through providing an accessible, reproducible and customisable set of tools. It builds on existing packages (matplotlib, pandas) to enable geochemists new to Python to hit the ground running, and encourages development of transferable digital skills. Features include:

- pyrolite.geom
  Transforming geochemical data
- pyrolite.mineral
  Mineral endmember calculation
- pyrolite.lattice
  Lattice strain calculation
- pyrolite.comp
  Compositional data transformations
- pyrolite.plot
  Ternary, spider, density diagrams and more. Templated plots (e.g. TAS, Pearce diagrams)
- pyrolite.util
  Utilities for scikit-learn, plotting, web interfaces, synthetic data, missing data, geological timescale & more

Documentation

Documentation for pyrolite is hosted at pyrolite.readthedocs.io, and includes a getting started guide, a set of examples for key features and detailed interface documentation.

Extensions

Extensions built around pyrolite which provide additional functionality beyond the core scope are also under development:

- pyrolite-meltutil
  An interface for conducting batch alphaMELTS calculations.
- pyrolite-datasource
  An interface to data from common geochemical repositories (e.g. EarthChem, currently a work in progress).

Community: Get Involved

pyrolite is developed for and by the geochemistry community. Contributions to the project are encouraged, and contributions of all forms are welcomed (e.g. code, documentation, bug reports and feature requests). Contributors to the project are recognised in the project contributors list.

pyrolite has an online community forum (gitter.im/pyrolite/community), and we’re happy to help you get up and running, answer questions and help with troubleshooting.

REFERENCES

[2] Hall, M.N.H., 1992. Orthogonal polynomial decomposition used to parameterise RHEE profile data using polynomial weights (or ‘lambdas’), which can be effectively used to quantitatively compare RHEE profile ‘shapes’.

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