



pyrolite: Python for geochemistry



@metasomite

Morgan Williams | 2021-03-19

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Australia's National Science Agency



Workshop - Intro

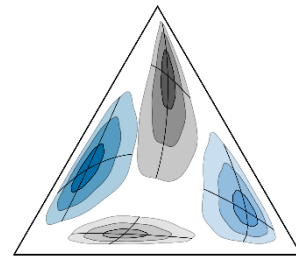
Facilitators:

- Morgan Williams (CSIRO)
- Hayden Dalton (U. Melb)
- Louise Schoneveld (CSIRO)

1. What is pyrolite? Why does it exist?
2. Core functions:
 - Handling geochemical data
 - Visualisation
 - Putting geochem data to work
3. Installation, Ecosystem & Tools
4. Get Involved
5. **Demonstration**
 - *Starting with some basics*

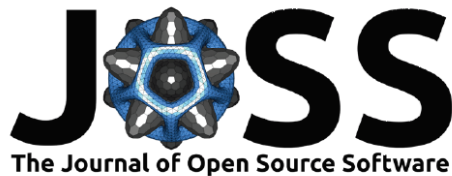


What is pyrolite?



- A set of tools for working with geochemical data
- An open source Python package (a bundle of reusable code)
- A project under active development, aiming to eventually be community-driven
- Part of a broader ecosystem of interoperable tools within the scientific Python ecosystem





pyrolite: Python for geochemistry

Morgan J. Williams¹, Louise Schoneveld¹, Yajing Mao², Jens Klump¹, Justin Gosses³, Hayden Dalton⁴, Adam Bath¹, and Steve Barnes¹

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DOI: [10.21105/joss.02314](https://doi.org/10.21105/joss.02314)

Software

- [Review](#) ↗
- [Repository](#) ↗
- [Archive](#) ↗

`pyrolite` is a Python package for working with multivariate geochemical data, with a particular focus on rock and mineral chemistry. The project aims to contribute to more robust, efficient and reproducible data-driven geochemical research.



What's the bigger idea?

Encouraging a programmatic approach to geochemical data analysis:

- Defining explicit workflows
- Reproducibility and reuse of research code
- Interoperability and automation
- Scalability and flexibility

To support this:

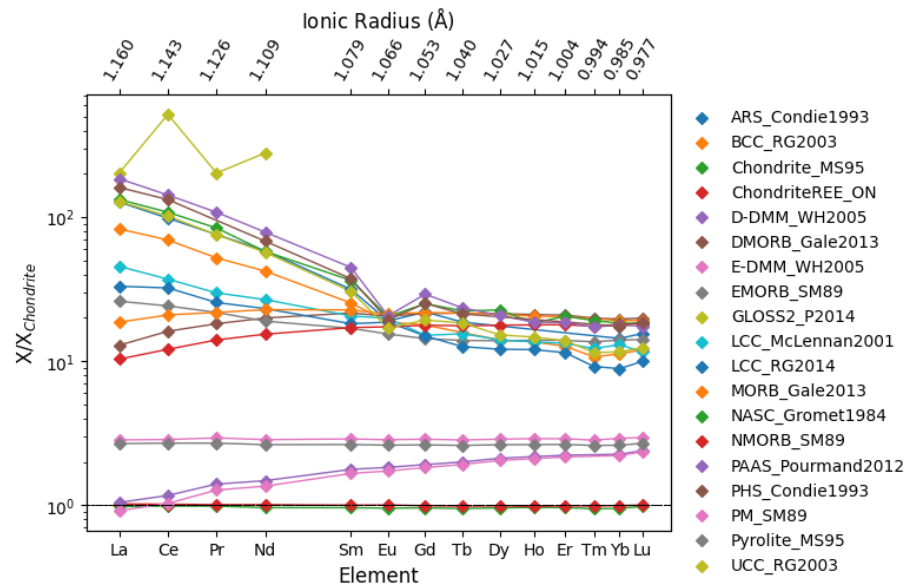
- Accessibility
- Community
- Education



pyrolite's Core Features

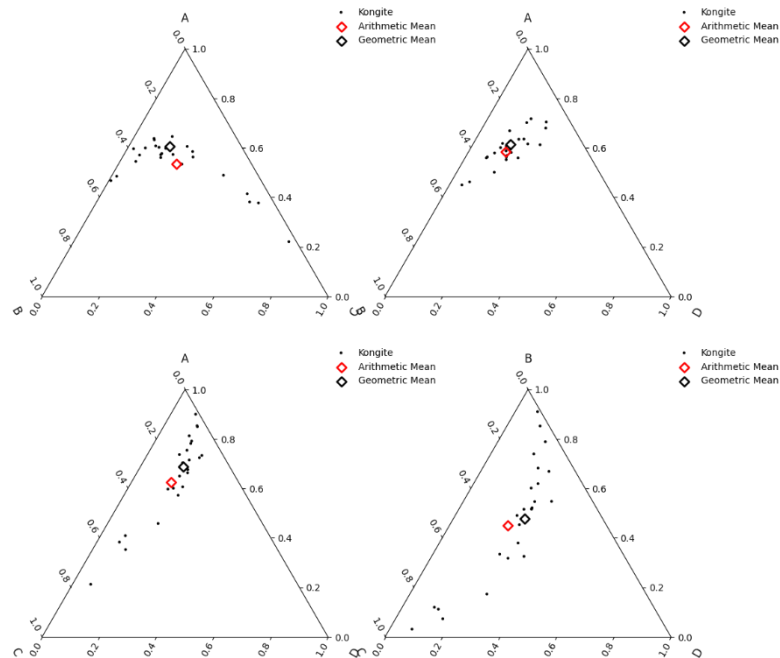
Handling Geochemical Data

- Transformation (elements, oxides, minerals, normalization)
- Reference compositions and mineral composition databases



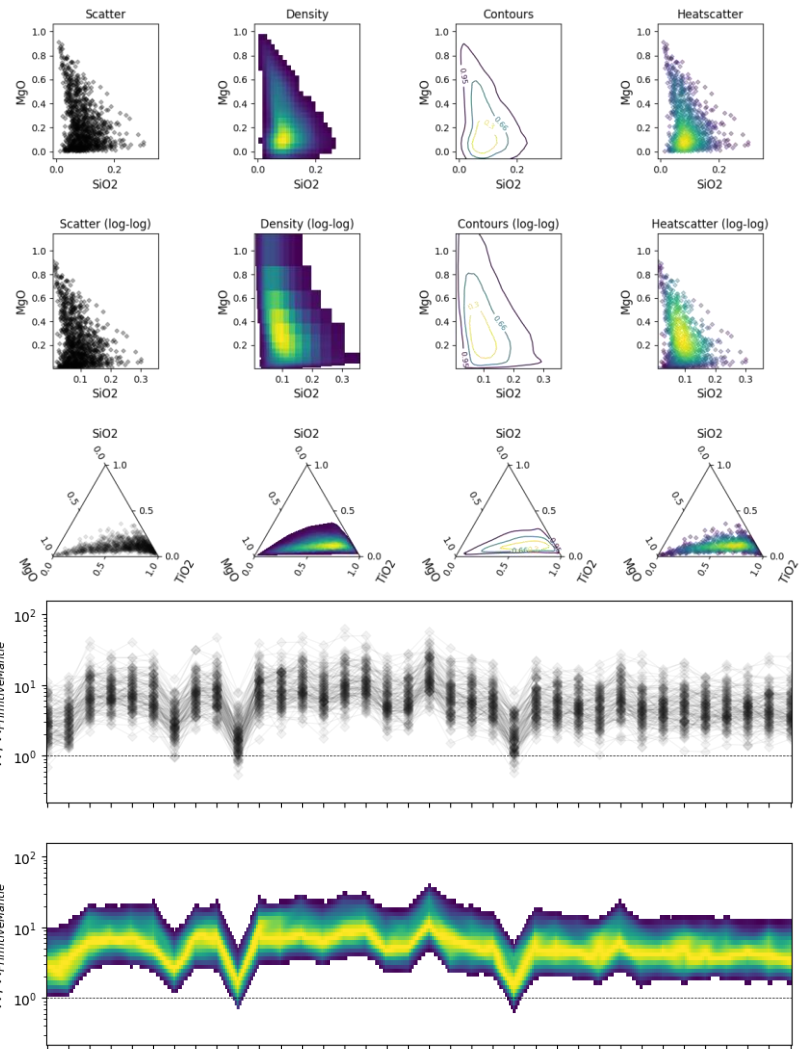
Handling Geochemical Data

- Transformation (elements, oxides, minerals, normalization)
- Reference compositions and mineral composition databases
- Compositional data – logratio transforms!
- Provide some specialized functionality to complement general tools
- Linking all of this directly to your dataset (data-centric, via Pandas)



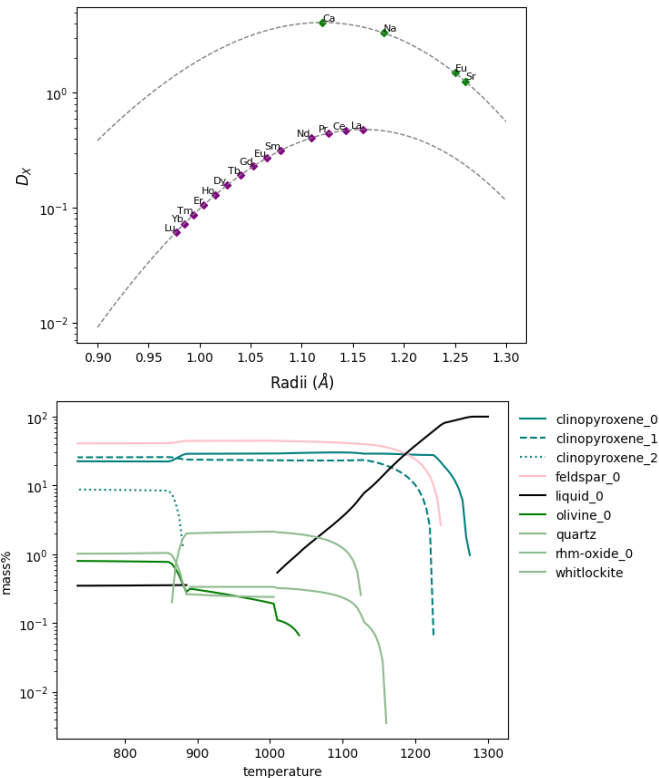
Visualisation

- Ternary diagrams
- Spider diagrams
- Addressing overplotting with data density-based visualisation methods
- Interface reflects the tools it's built on top of (e.g. matplotlib) in order to be interoperable
- Highly customisable



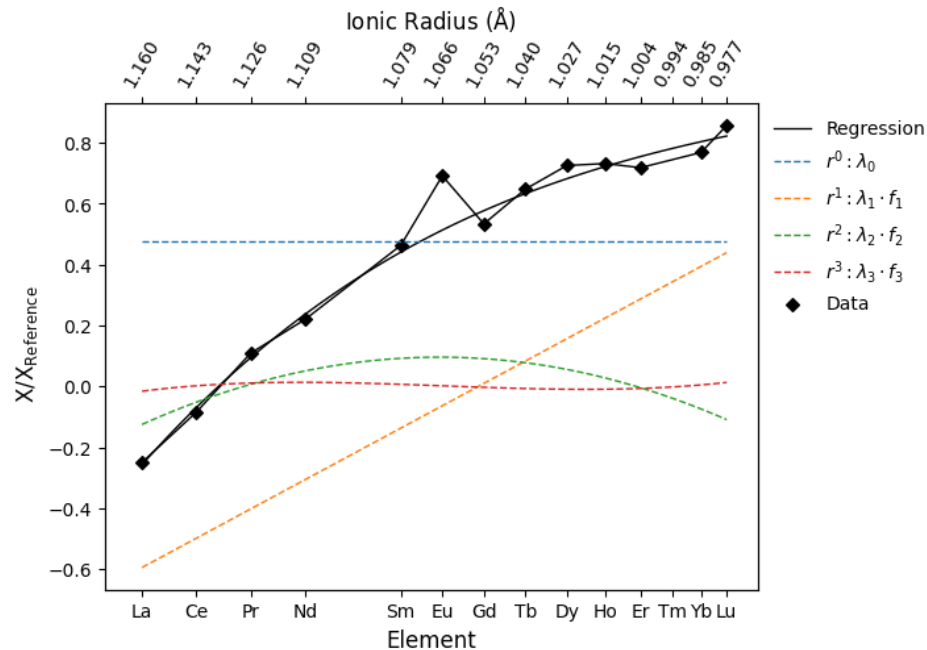
Linking Geochem Data to Modelling and ML

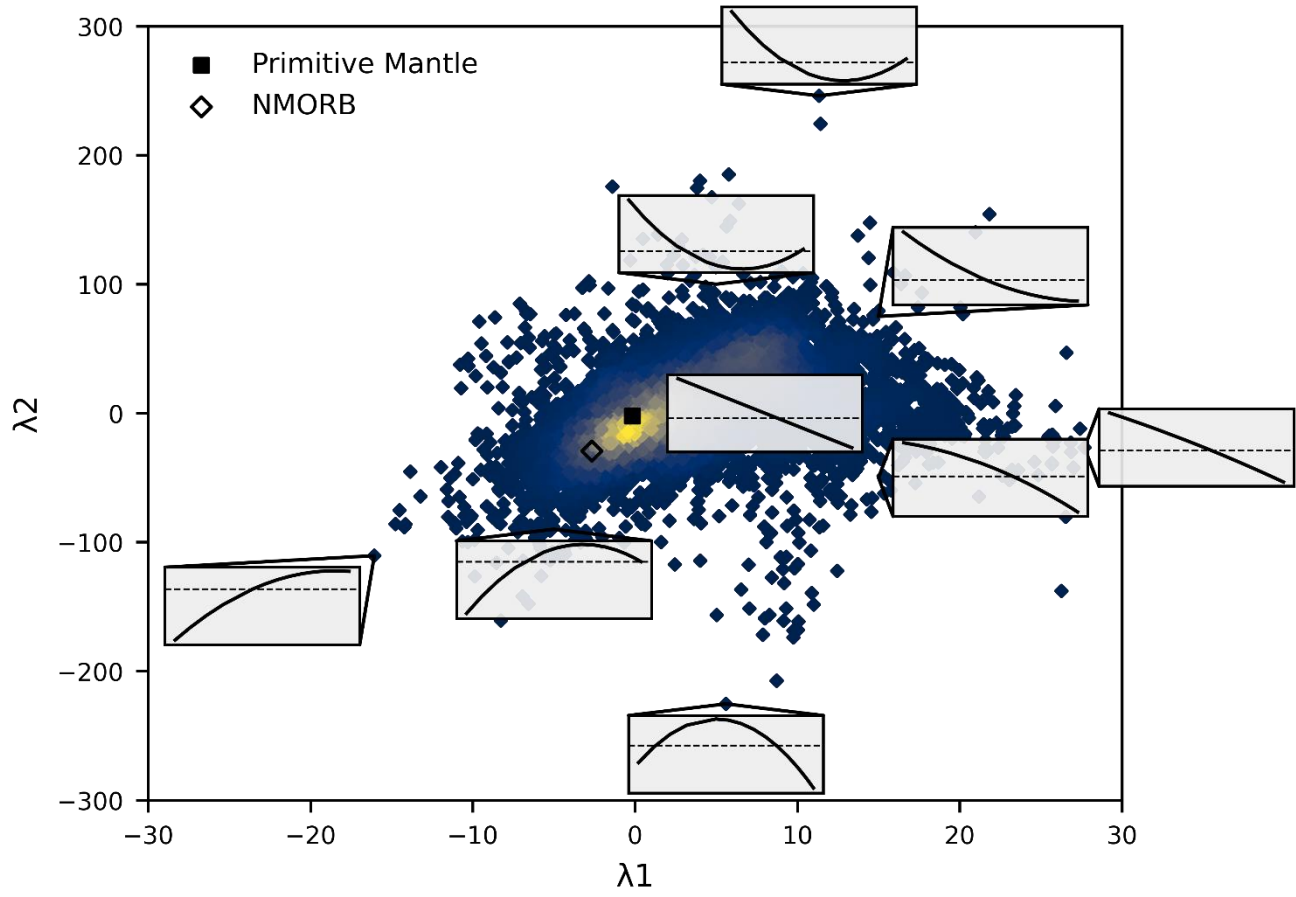
- To get the most out of our geochemical data, we'll need to be able to link it to a variety of different tools
 - Modelling (e.g. lattice strain, alphaMELTS)
 - Machine learning
- The scientific Python ecosystem comes with 'batteries included'



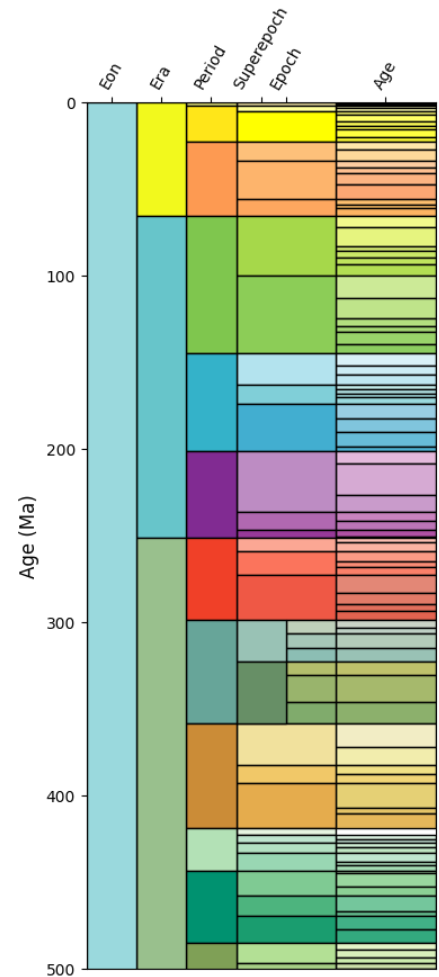
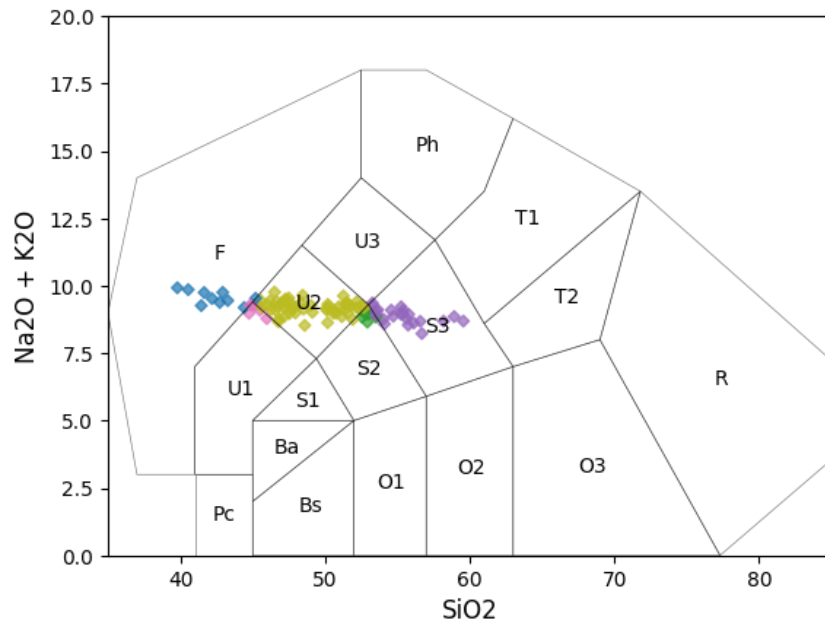
Lambdas: Parameterising REE Profiles

- Quantitative description of REE profiles closely linked to geological processes
- Customisable implementation of orthogonal polynomial regression, after O'Neill (2016)
- Tetrads, anomalies, fit measures and parameter uncertainties released in v0.3.0





And a range of other utilities...





Extensions

pyrolite-meltsutil

- Working with alphaMELTS and its outputs
- Automating batch calculations over a grid of parameters and compositions.

pyrolite-datasource (not yet released)

- Directly accessing data from GEOROC and EarthChem



Installation, Ecosystem & Tools



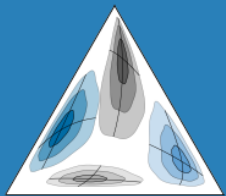
```
> pip install pyrolite
```

Pyrolite is hosted on the Python Package Index (PyPI), and each new release (\approx every few months) will be uploaded there and on GitHub. In the future it will also likely be released via conda-forge.



Docs

pyrolite.rtfd.io



develop

GETTING STARTED

- Installation
- Getting Started

Examples

- Plotting Examples
- Geochemistry Examples
- Compositional Data Examples
- Utility Examples

Tutorials

- Citation

DEVELOPMENT

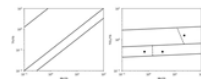
- Development
- Changelog
- Future
- Code of Conduct
- Contributing
- Contributors

REFERENCE

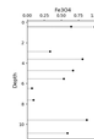
- API

Plotting Examples

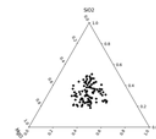
pyrolite provides some functionality for basic plotting of geochemical data in the form of spidergrams (`pyrolite.plot.spider`), ternary diagrams (`pyrolite.plot.tern`) and density diagrams (i.e. 2D histograms, `pyrolite.plot.density`).



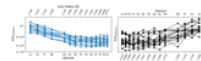
Plot Templates



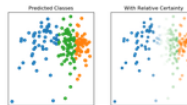
Stem Plots



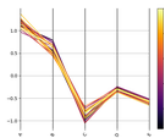
Ternary Plots



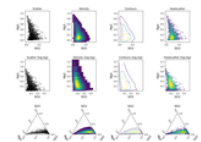
REE Radii Plots



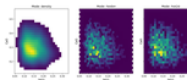
Using Manifolds for Visualisation



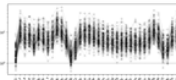
Parallel Coordinate Plots



Heatscatter Plots



Density and Contour Plots



Spiderplots & Density Spiderplots



GitHub

- Code repository
- Issue Tracker
- Version archive (also on Zenodo)

morganjwilliams / pyrolite

<> Code Issues Pull requests Actions Projects Wiki Security Insights Settings

master 2 branches 48 tags Go to file Add file + Code

morganjwilliams Merge branch 'release/0.3.0' ✓ October 3 days ago 1,709 commits

github	Add Docs Build Test Workflow to Actions	2 months ago
binder	Remove docs build from binder config	17 months ago
docs	Remove Todo from changelog - these can stay in Issues.	3 days ago
paper	Update pyOpenSci Submission Notes	13 months ago
pyrolite	Rx parse_sigmas type, remove unused plot.parallel func	3 days ago
test	Small formatting updates, raw strings for escape sequences	3 days ago
.codacy.yml	Add contributing.md to codacy exclude	10 months ago
.coveragerc	Edit workflow for parallel coveralls	2 months ago
.github	Minor changes to accessory files	7 months ago
.gitignore	Minor changes to accessory files	7 months ago
.readthedocs.yml	Add pdf output for md	16 months ago
CHANGELOG.md	Docs Refactor	17 months ago
CODE_OF_CONDUCT.md	Update markdown pointer to docs CoC	13 months ago
CONTRIBUTING.md	Update contributing.md formatting	10 months ago
LICENSE	Update to Hybrid MIT BSD CSIRO License	3 years ago
MANIFEST.in	Add data/_config to the manifest	8 months ago
README.md	Edit README Badge Links	2 months ago
environment.yml	Rx spider type	2 months ago
setup.cfg	Add xml coverage report	13 months ago
setup.py	Add pypi to requirements	4 months ago
versioneer.py	The Beginning	3 years ago

README.md

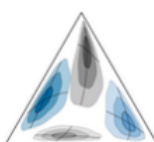
pyrolite

Docs [openings](#) [PyOpenSci](#) [Peer Review](#) [DOI: 10.1101/2020.02.04.000000](#)
License [CSIRO BSD/MIT License](#) [TryItOut With Binder](#) [Cite on GitHub](#)

pyrolite is a set of tools for making the most of your geochemical data.

The python package includes functions to work with compositional data, to transform geochemical variables (e.g. elements to oxides), functions for common plotting tasks (e.g. spiderplots, ternary diagrams, bivariate and ternary density diagrams), and numerous auxiliary utilities.

pyrolite is principally developed for use in geochemical research, but is also well suited to being incorporated into university-level geochemistry and petrology classes which wish to include a little Python. The documentation is continually evolving, and more examples and tutorials will gradually be added (feel free to request features or examples; see [Contributing](#) below).



About

A set of tools for getting the most from your geochemical data.

[pyrolite.readthedocs.io](#)

[data-science](#) [chemistry](#) [geochemistry](#) [geochemical-data](#) [csiro](#) [ternary-diagrams](#)

Readme

View license

Releases [0.3.0](#) (Latest) 3 days ago

+ 47 releases

Packages

No packages published

[Publish your first package](#)

Contributors [3](#)

[morganjwilliams](#) Morgan Williams

[kaarelmaand](#) Kaarel Mänd

[lavender22](#) Louise Schoneveld

Languages

Python 97.5% [View details](#) [View details](#)



Get Involved

- Want help getting started?
- Find something which looks like a bug?
- Want to be able to do something, but not sure how/if its possible?
- Want to get involved with the project, or have ideas where it should go?
- Keen to make the project more sustainable?

- Want a sticker?
Catch me when we get back to in-person conferences..

Discussion:

gitter.im/pyrolite/community

Bugs and Features:

github.com/morganjwilliams/pyrolite



Some Perspectives on Getting Started

- Start where you are. For new coders, it'll take a while to get used to. Don't expect to learn everything overnight.
- Play around with the examples, then try working with your own data. Having a project or objective in mind helps with the learning process!
- I still have to look up & copy-paste lots of things, even for my own code. This probably won't change!



Quick Demo

- Python Basics
- Pulling in and transforming some data
- Visualisation
- Working with mineral data
- lambdas

Play along:

tinyurl.com/202103-MQ-pyrolite

The screenshot shows a GitHub repository page for 'pyrolite Workshop - Macquarie University Geochemistry Group'. The repository is owned by 'morganjwilliams' and has 14 commits. The main branch is 'develop', which is 10 commits ahead of 'main'. The repository contains a 'data' directory, 'notebooks', '.gitignore', 'LICENSE', and 'README.md'. The README.md file is displayed, showing the repository's purpose: 'This repository contains the content for the 2021-03-19 pyrolite workshop for Macquarie University's Geochemistry Group'. The repository is licensed under MIT and has a 'docs' link pointing to 'passing'. The repository is also linked to a Gitter chat and a Twitter account '@metasomite'.

Repo: github.com/morganjwilliams/202103-MQ-pyrolite-workshop





Thank you



@metasomite

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Australia's National Science Agency

pyrolite Contributors:

- Hayden Dalton
- Louise Schoneveld
- Adam Bath
- Yajing Mao
- Justin Gosses
- Kaarel Mand
- Laura Miller
- Steve Barnes
- Lucy Mathieson



This is the first official pyrolite workshop
we've run! How'd we go?

Q&A, Feedback