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pyrolite: An Open Source Toolbox for Geochemical Data Analysis and Visualisation

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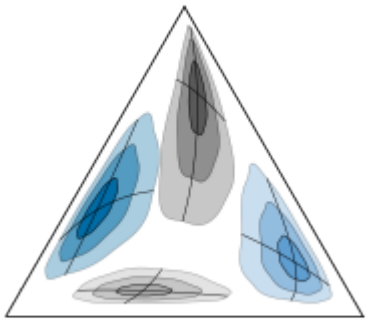

pyrolite is a set of tools for working with geochemical data. The open source Python package provides functionality for transforming, analysing and visualising geochemical data, and aims to allow new users to get off the ground quickly. The project encourages a programmatic approach to geochemical data analysis, allowing the explicit definition of data analysis workflows supporting increased reproducibility and reuse. The package also provides an interface for linking geochemical data to visualisation, modelling, automation and machine learning workflows enabled by the broader scientific Python ecosystem. This presentation will provide a series of demonstrations of pyrolite's functionality and a few key use cases including machine geochemical classification/discrimination problems.

pyrolite provides foundational capability for geochemical transformation and scaling, compositional data analysis and visualisation (e.g. spider, ternary and data density diagrams). It also includes implementations of a series of commonly used models and novel algorithms including lattice strain models [1], 'lambdas' for Rare Earth Element pattern parameterisation [2] and spatiotemporal bootstrap resampling [3]. A database of reference compositions for common geological reservoirs (e.g. Chondrite, primitive mantle) and a database of endmember compositions of common rock forming minerals are included to provide relevant geochemical context. The pyrolite documentation contains a gallery of examples and tutorials in addition to API documentation (describing the range of functions and classes).

pyrolite is under active development and is open to new contributors. We hope to foster a growing community of users and contributors to ensure the long-term sustainability and usefulness of the project. The package has been openly peer-reviewed and published through pyOpenSci and the Journal of Open Source Software [4].

[1] O'Neill (2016), *Journal of Petrology* 57, 1463–1508.

[2] Blundy & Wood (1994), *Nature* 372, 452.

[3] Keller & Schoene (2012), *Nature* 485, 490–493.

[4] Williams, Schoneveld, Mao, Klump, Gosses, Dalton, Bath, & Barnes (2020), *Journal of Open Source Software* 5, 2314.