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Developing reusable tools for geochemical data in Python: the pyrolite roadmap

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pyrolite is a set of tools for working with geochemical and mineralogical compositional data. The open-source package is written in Python, and contains a range of functionality for transforming, analysing and visualizing compositional data [1]. It is designed to be used in a programmatic manner, allowing the explicit definition of data analysis workflows and integration with other visualisation, modelling, automation, and machine learning tools within the broader scientific Python ecosystem. pyrolite focuses on providing a set of configurable and reusable tools, using an interface built upon the core packages used for data analysis in Python for familiarity (including Pandas [2] and matplotlib [3]), aiming to enable users to achieve desired outputs quickly and repeatedly. The associated documentation consists of a gallery of examples and tutorials in addition to API documentation. This documentation is supplemented by further examples of applications from associated workshops targeted at learners with little to no previous Python experience.

The development of pyrolite has continued steadily since its initial release, with the number of both users and contributors steadily growing over this time. Recent development has included a Python implementation of a CIPW Normative mineralogy algorithm [4] and a range of standardised rock and mineral classification diagrams (including for ternary spaces). A number of additional features and enhancements remain on the development roadmap, including interactive visualization options, improved automatic handling of units, expansion of internal reference datasets (e.g. for mineral compositions), and a number of additional diagram templates. This presentation will summarize the current functionality of pyrolite, highlight some of the recent additions and contributions, and discuss prototype implementations of some planned features.

References

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