

Thermodynamic Modelling and Trace Element Partitioning as Predictive Tools for REE-Enrichment in Alkaline-Silicate Igneous Systems

Corinne Frigo¹, Owen Weller¹, Caroline Soderman¹, Charles Beard², Teresa Ubide³

¹Department of Earth Sciences, University of Cambridge, United Kingdom, ²Department of Earth Sciences, Utrecht University, Netherlands, ³School of the Environment, University of Queensland, Australia

The increasing demand for rare earth elements (REEs) in green technologies calls for more effective strategies to identify environments where they may have been concentrated. Alkaline-silicate igneous systems (and associated carbonatites) are key hosts of REE deposits, yet many contain no economic mineralisation. This study evaluates the potential of coupling thermodynamic phase equilibria modelling with empirical trace element partitioning equations to predict optimal conditions for residual enrichment of the REE during the crystallisation of alkaline-silicate systems.

We test this approach using a case study of the Erongo Complex in Namibia, focusing on a suite of late intrusive plugs of basanite to foidite composition [1]. Using the bulk composition of the most primitive basanite as a starting melt, we simulate batch and fractional crystallisation at varying pressure-temperature conditions with the software MAGEMin [2] and a new thermodynamic dataset for alkaline-silicate systems [3]. These simulations predict melt and mineral equilibria, modal abundances, and compositions, which we test against observations from natural samples. Empirical partitioning equations [e.g., 4–6] are used to estimate REE concentrations in melt and coexisting mineral phases. These results are compared with whole-rock REE data and LA-ICP-MS maps of zoned clinopyroxene grains, known as effective recorders of melt evolution [4]. By confirming that major and trace element trends observed in nature can be reproduced, the thermodynamic models can be used to forward model the ‘sweet spot’ for optimal REE enrichment [7].

References:

- [1] Trumbull RB et al. (2003) *J. Petrology* 44
- [2] Riel N et al. (2022) *Geochem. Geophys. Geosyst.* 23
- [3] Weller O et al. (2024) *J. Petrology* 65
- [4] Beard C et al. (2019) *J. Petrology* 60
- [5] Baudouin C et al. (2020) *Contrib. Min. & Pet.* 175
- [6] Salazar-Naranjo AF & Vlach SRF (2025) *Chem. Geo.* 677
- [7] Soderman et al. (2025) *Nature Geoscience*, doi:10.1038/s41561-025-01695-3