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Predicting Global Mantle Oxygen Fugacity Using Machine Learning

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Clinopyroxene is a major Fe^{3+}-bearing rock-forming mantle mineral across pressure-dependent plagioclase-spinel-garnet field. However, clinopyroxene remains underutilized in mantle oxygen fugacity estimation despite its potential as oxybarometer first suggested by Luth and Canil (1993). To address this gap, we applied machine learning to: 1) Develop a more generalized model without prior clinopyroxene species classification required by Huang et al. (2022); 2) Update clinopyroxene-only thermobarometer of Qin et al. (2024), based on an expanded database (2369 entries) of clinopyroxene composition, temperature (T), and pressure (P); 3) Create the clinopyroxene oxybarometer trained on 1185 entries incorporating clinopyroxene composition, *T*, *P*, oxygen fugacity, and predicted Fe^{3+} content and $Fe^{3+}/\Sigma Fe$ ratio. We prioritize models with outstanding scores on test sets, then discard models showing either significant discrepancy between training and validation/test scores or sharp performance decline from validation to test sets - both indicative of overfitting.

Applied to 9,848 global mantle clinopyroxenes from xenoliths, ophiolites, and massifs, the models replicate lateral oxygen fugacity variations across diverse tectonic settings, aligning with spinel/garnet-based methods. The machine-learning approach extends predictions beyond well-studied regions (e.g., Kaapvaal, Siberia) to previously understudied areas including Baltica Craton, North Atlantic Craton, New Caledonia, Philippines ophiolites, and Alps, Tibet massifs where Fe^{3+} data spinel or garnet xenoliths are limited. The gradient of oxygen fugacity-depth profiles for each craton ranges from 0.8-1.1 log units per GPa up to ~240 km depth without significant variation over long-term evolution since ~1.18 Ga. This machine learning approach expands spatial coverage and depth resolution of mantle redox studies.

Reference:

Huang, W.-h., Lyu, Y., Du, M.-h., He, C., Gao, S.-d., Xu, R.-j., et al. (2022). Estimating ferric iron content in clinopyroxene using machine learning models. *American Mineralogist, 107*(10), 1886-1900. https://doi.org/10.2138/am-2022-8189

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Qin, B., Ye, C., Liu, J., Huang, S., Wang, S., & ZhangZhou, J. (2024). Mapping Global Lithospheric Mantle Pressure-Temperature Conditions by Machine-Learning Thermobarometry. *Geophysical Research Letters, 51*(7), e2023GL106522. https://doi.org/10.1029/2023GL106522