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Estimating ferric iron content in clinopyroxene using machine learning models

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Clinopyroxene ferric iron content is an important consideration for garnet-clinopyroxene geothermometry and estimations of water storage in the Earth's interior, but remains difficult and expensive to measure. Here, we collect 407 natural clinopyroxenes with $Fe^{3+}/\sigma Fe$ measured by Mössbauer spectroscopy and develop seven classic algorithms and machine learning methods to estimate $Fe^{3+}/\sigma Fe$ in clinopyroxene using major element data from electron microprobe analyses. Our results suggest that ensemble learning algorithms (random forest and Extra-Tress) perform better than principal component analysis-based elastic net polynomial, artificial neural network, artificial neural network ensemble, decision trees, and linear regressions. The models trained by the whole dataset of clinopyroxene spanning a wide compositional range achieve root-mean-square-errors on the test dataset ranging from 0.071 to 0.089. Using sub-dataset excluding clinopyroxene in spinel peridotite and omphacite in eclogite to train new models decreases prediction errors by 30-40%, with root-mean-square-errors on the test dataset ranging from 0.051 to 0.078. The prediction for clinopyroxene in spinel peridotite is improved by training models that incorporating compositional data on coexisting spinel. All of our models show much greater precision than traditional calculation methods based on charge conservation. The application of our models to garnet-clinopyroxene geothermometry greatly improves temperature estimates, achieving uncertainties of ±50 °C, compared with uncertainties of ±250 °C using previous models assuming all Fe as Fe^{2+} or calculating Fe^{3+} by charge conservation. Differences in the ferric iron contents, as calculated using the machine learning models, of clinopyroxenes that did or did not experience hydrogen diffusion during their crystallization from basaltic magma support a redox-driven mechanism for hydrogen diffusion in clinopyroxene.