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Quartz trace elements as petrogenetic indicators: a machine learning approach

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Quartz (SiO_2) is the second most abundant mineral in the upper silicic crust and one of the few mineral phases that commonly occur across magmatic, hydrothermal, metamorphic, and sedimentary environments. In silicic magmatic systems, quartz is almost always present, making it a key archive of information for reconstructing magmatic and volcanic processes. Trace elements in quartz have long been used to infer crystallization conditions and magma evolution. However, their application has been limited by the fact that only four elements are consistently measurable in most quartz crystals: Ti, Al, Ge, and Li, resulting in overlapping compositional fields that are difficult to resolve using traditional discrimination approaches. In recent years, the development of machine learning algorithms has provided Earth scientists with a multitude of new possibilities for reinterpreting existing trace element datasets, allowing for the identification and classification of chemical signatures previously considered too subtle to resolve. In this study, we apply machine learning to investigate the trace element composition of quartz. We built a stacked model, combining k-nearest neighbors (kNN), random forest, and gradient boosting. Our model allows for classification of quartz crystals based on magmatic environment (plutonic, volcanic, pegmatitic, or hydrothermal) and chemical affinity (A-, S-, I-type melts). We validated our model by testing two datasets: (1) a dataset of quartz from the Tava Sandstone (Pikes Peak Batholith, CO, USA), a sedimentary unit with well-established quartz provenance; (2) a dataset of combined Australian granites. The model correctly identified quartz provenance in both test datasets. These findings demonstrate that our model holds potential not only for deconvoluting overprinted/multi-stage complex chemical histories but also for supporting provenance studies in sedimentary geology.