Goldschmidt 2024 Abstract
https://doi.org/10.46247/gold2024.23779

Automated Mineral Identification by Stoichiometry (MIST): A Tool for Geochemical Dataset Standardization

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Identifying minerals is a prerequisite to interpreting geologic history from samples. Various techniques for mineral identification are available, but one method commonly used for individual grains or crystals in a sample is to obtain high-resolution geochemical information of the grain and compare element ratios to known minerals, i.e., stoichiometry.

We developed MIST (Mineral Identification by Stoichiometry) as a first-principles-based computational algorithm to identify geochemical observations with stoichiometric elemental ratios that match real-world compositions. Identifying minerals by stoichiometry works when the geochemical measurement spot size is smaller than the size of the mineral. Beyond this requirement, stoichiometric rules are agnostic to the source of geochemical data. MIST uses normalized oxide weight percentages and stoichiometric ratios between elements in a detailed decision tree approach to identify mineral phases using recognized mineral group hierarchies. The approach incorporates tolerances tailored to the imperfections and elemental substitutions common in real-world minerals. When an observation matches a mineral species, we output the name of the mineral according to IMA rules and a detailed stoichiometric mineral formula. The algorithm has been tested on well over 2000 mineral compositions and currently identifies 250 mineral species with >95% accuracy. MIST is free to use via an online API at mist.rice.edu.

Data quality testing and standardization is a significant area of development in geochemical databases and compilations of geochemical results. MIST can rapidly standardize mineral chemistry datasets by recognizing when a geochemical measurement stoichiometrically matches a mineral. For example, we tested 222,543 geochemical compositions classified as olivine in the GEOROC chemical database. After filtering for SiO_2 wt.% > 0, we found that 21% matched a pure olivine (forsterite or fayalite) composition; 38% were chemically consistent with the antigorite/lizardite/chrysotile group of alteration minerals. Accuracy is a known issue with databases that collect decades of data, but if each individual user must filter the datasets themselves, they likely select compositions based on the individual's perception of the tolerance of real mineral variations; MIST can standardize this filtering process, preparing datasets for better use in research projects and as training datasets for machine learning models.

MIST
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