Identifying biogenic signatures in pyrite by combining sulfur isotopes and trace elements analyses

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Current methods for identifying signatures of past life are challenged by the rarity of unambiguous fossils and difficulties associated with preservation of ancient organic materials. However, minerals that form through direct or indirect biological processes while incorporating trace elements in concentrations that are proportional to those in the surrounding fluid provide details about past environmental conditions and about the life present at the time of formation. In-situ geochemical techniques for analysing discrete mineral grains can minimize the overprinting effects potentially present in bulk-sample techniques. Here we show how in-situ analyses of trace elements (TE) and sulfur isotopes of pyrite by LA-ICPMS and SIMS, respectively, can help us interpret evidence for life in the rock record. Sedimentary pyrite is inextricably linked to life through microbial sulfate reduction, and biological processes affect the TE abundance and sulfur isotope composition of pyrite. Importantly, sedimentary pyrite has TE and sulfur isotope ($\delta^{34}S$) properties that differ from those of hydrothermal and magmatic pyrite. We have coupled trace element and sulfur isotope data from 400 pyrite measurements from diverse sedimentary, hydrothermal, and magmatic deposits. Random Forest (RF), a machine learning algorithm with proven value in statistical classification, was used to classify pyrite into deposit types.

We show than when TE and $\delta^{34}S$ are both used, sedimentary pyrite is correctly identified with 94% accuracy (F1 score). However, less accurate predictions are observed when classifying pyrite using TE and $\delta^{34}S$ values separately. The resulting average F1 scores are 93% and 83%, respectively. Thus, our results demonstrate the strength that comes with coupled TE and $\delta^{34}S$ data for effectively identifying sedimentary pyrite and thus a likely biological contribution. Through validation and calibration of our data, we will increase our ability to recognize pyrite linked to microbial life, providing a novel window in the search for ancient and distant biology. The goal is to apply the approach across a wide range of samples from well-constrained modern terrestrial analogues, thus expanding the reach of the analytical and statistical techniques within the astrobiological community including applications to Mars research. If successful, this method can serve as an alternative to traditional rock-bound biosignatures via techniques that are relatively routinely applied.