

Abstract

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Chemometric evaluation of time-of-flight secondary ion mass spectrometry data of minerals in the frame of future *in situ* analyses of cometary material by COSIMA onboard ROSETTA.

Chemometric data evaluation methods for time-of-flight secondary ion mass spectrometry (TOF-SIMS) have been tested for the characterization and classification of minerals. Potential applications of these methods include the expected data from cometary material to be measured by the COSIMA instrument onboard the ESA mission ROSETTA in the year 2014.

Samples of the minerals serpentine, enstatite, olivine, and talc have been used as proxies for minerals existing in extraterrestrial matter. High mass resolution TOF-SIMS data allow the selection of peaks from inorganic ions relevant for minerals.

Multivariate cluster analysis of peak intensity data by principal components analysis and the new method CORICO showed a good separation of the mineral classes. Classification by k nearest-neighbor classification (KNN) or binary decision trees (CART method) results in more than 90% correct class assignments in a leave-one-out cross validation.