

Abstract

J. Chemometrics, 2020, e3218, 1-8 (2020)

Varmuza K., Filzmoser P., Fray N., Cottin H., Merouane S., Stenzel O., Paquette J., Kissel J., Briois C., Baklouti D., Bardyn A., Siljeström S., Silen J., Hilchenbach M.:

Composition of cometary particles collected during two periods of the Rosetta mission - multivariate evaluation of mass spectral data.

Open access: <https://doi.org/10.1002/cem.3218>

The instrument COSIMA (COmetary Secondary Ion Mass Analyzer) onboard of the European Space Agency mission Rosetta collected and analyzed dust particles in the neighborhood of comet 67P/Churyumov-Gerasimenko. The chemical composition of the particle surfaces was characterized by time-of-flight secondary ion mass spectrometry.

A set of 2213 spectra has been selected, and relative abundances for CH-containing positive ions as well as positive elemental ions define a set of multivariate data with nine variables. Evaluation by complementary chemometric techniques shows different compositions of sample groups collected during two periods of the mission. The first period was August to November 2014 (far from the Sun); the second period was January 2015 to February 2016 (nearer to the Sun).

The applied data evaluation methods consider the compositional nature of the mass spectral data and comprise robust principal component analysis as well as classification with discriminant partial least squares regression, k -nearest neighbor search, and random forest decision trees.

The results indicate a high importance of the relative abundances of the secondary ions C^+ and Fe^+ for the group separation and demonstrate an enhanced content of carbon-containing substances in samples collected in the period with smaller distances to the Sun.