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Rosetta/COSIMA: Principal Component Analysis Applied to Time-of-Flight Secondary Ion Mass Spectra

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1. Abstract

The **CO**metary **S**econdary **I**on **M**ass **A**nalyser (COSIMA) on board ESA's Rosetta spacecraft is a high-resolution ($m/\Delta m \approx 2000$ at $m = 100\,\mathrm{amu}$; from FWHM) time-of-flight mass spectrometer dedicated to the in-situ analysis of ($10\,\mu\mathrm{m}$ and larger) dust grains in the coma of comet 67P/Churyumov-Gerasimenkov. COSIMA is equipped with a primary indium ion source, a high resolution mass spectrometer, an optical microscope and a sample manipulation unit [Kissel et al., 2007]. Beginning in 2014, after Rosetta's arrival at the comet, COSIMA will collect cometary dust grains on metal targets, will investigate the exposed targets with an optical camera and will measure mass spectra generated by ion bombardement. A flight spare unit of COSIMA (reference model, RM) is located at Max-Planck-Institut für Sonnensystemforschung (MPS), Katlenburg-Lindau. The RM is a twin of the COSIMA flight instrument and is used for laboratory calibration measurements.

Here we present results from an ongoing laboratory calibration campaign with the COSIMA RM. We have prepared cometary dust analogue samples (powder with grain size $\approx 10\,\mu\mathrm{m}$) from natural and synthetic minerals (pyroxene, olivine, hydrous silicates, sulfide, etc.), which – except for hydrous minerals – have been identified in cometary matter [Burchell and Kearsley, 2009]. A large number of time-of-flight mass spectra of these samples was measured with the COSIMA RM. Spectra from the different mineral samples show characteristic mass lines, grossly reflecting the mineral composition. With Principal Component Analysis (PCA) we are able to separate the spectra of our mineral samples into individual groups. Thus, PCA – together with other chemometric techniques [Engrand et al., 2006, Varmuza et al., 2011] – is a useful tool for the classification of COSIMA mass spectra. Further experiments have to show whether it can also be used for the classification of organic compounds and mixtures of, e.g., organic compounds and mineral grains.

References

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