An automatic pipeline processing software for secondary ion time-of-flight mass spectra of Rosetta/COSIMA

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Abstract

The COrryhotary Secondary Ion Mass Analyser (COSIMA) onboard the Rosetta orbiter will collect and analyse dust grains in the coma of comet 67P/Churyumov-Gerasimenko beginning in 2014. COSIMA is a high-resolution time-of-flight mass spectrometer (m/Δm ≈ 2000 at m ≈ 100 amu), from FWHM [5]. We expect to obtain thousands of COSIMA mass spectra during the entire Rosetta mission at the comet. In order to be able to handle and efficiently analyze such a large amount of data, we develop an automatic data processing software. The resulting data is a peak list, giving – for each peak identified in the spectrum – peak intensity, exact mass, suggested ion species, etc. This peak list will serve various purposes: 1) Identification of interesting spectra for subsequent more detailed evaluation, 2) Input for statistical multivariate analyses (e.g., Corioca, Principal Component Analysis [3]), 3) Input for further automatic data processing, like, e.g., intensity maps from COSIMA raster scans. We present the current status of our pipeline software and show examples for its application to COSIMA laboratory spectra.

Future Improvements

- Extensive testing required!
- Peak profiles of TOF-SIMS instruments are well-known for being non-Gaussian shaped. Peak fitting with a ‘standard’ profile derived from the spectrum itself (e.g., lines used in Figure 2) will be tested.
- Deconvolution of unresolved double peaks.
- Assignment of ion species: consider isotopic ratios, potential hydride contributions, organic compounds, etc. to improve peak assignment [3].
- Improve removal of instrumental artefacts (e.g., non-linearity correction for TDC, improved background determination).

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References