Characterisation of meteoritic samples with the Rosetta Cosima TOF-SIMS laboratory reference model – a covariance approach

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Abstract

The time-of-flight secondary ion mass spectrometer Cosima on board Rosetta will analyse cometary grains ejected off the nucleus of comet 67P/Churyumov-Gerasimenko from September 2014 onwards. In our effort to understand the composition and the history of these cometary grains, we study the characteristics of different meteorite samples with the Cosima reference instruments at the Max Planck Institute for Solar System Research, with the goal to separate individual compounds and their fragmentation patterns.

Different types of meteorite dust are prepared in the laboratory. Among these are one ordinary chondrite H4 (Ochansk), one unequilibrated ordinary chondrite H3 (Tieschitz), one carbonaceous chondrite CR (Renazzo), and a Martian shergottite (Tissint). Grains of sizes up to 100 μm are pressed into a blank gold metal target.

The grains are identified with the instrument microscope and positive and negative secondary ion mass spectra are accumulated on different positions on selected grains. The mass spectra comprise secondary ions up to mass 300 with reasonable detection efficiency and a mass resolution of 1400 @ 100 u. This mass resolution is sufficient to separate organic (hydrogen rich) molecule peaks from minerals or elemental mass peaks.

We are trying to assess how the covariances of count rates between different parts of the mass spectra, i.e. specific atomic and molecule peaks of a single meteorite, can be used to infer some properties of its constituents and how this differs between the different meteorites that show varying degrees of alteration. In a first step we look at the covariance and the correlation matrices S of the mass spectra for individual meteorite samples.

This will help us, after future analysis, to place the cometary grains into the proper compositional and evolutionary context within the various materials of the solar system.

Cosima, the COmetary Secondary Ion Mass Analyzer

is the time of flight secondary ion mass spectrometer on board Rosetta [1].

SIMS data are complex, representing the elements and molecules on the surface area analyzed by the primary ion beam. The interpretation of the spectra requires knowledge of the stable molecular ions as well as statistical methods analyzing and comparing mass spectra.

The spectra are taken from cometary analog and reference samples analyzed with the laboratory reference instrument of COSIMA [2,3] .

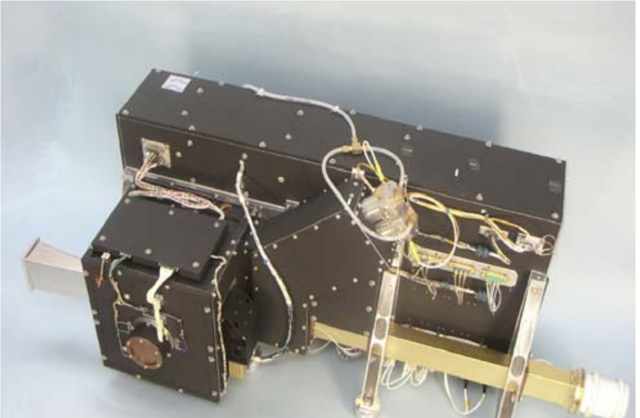

Figure1: Flight model of Cosima.

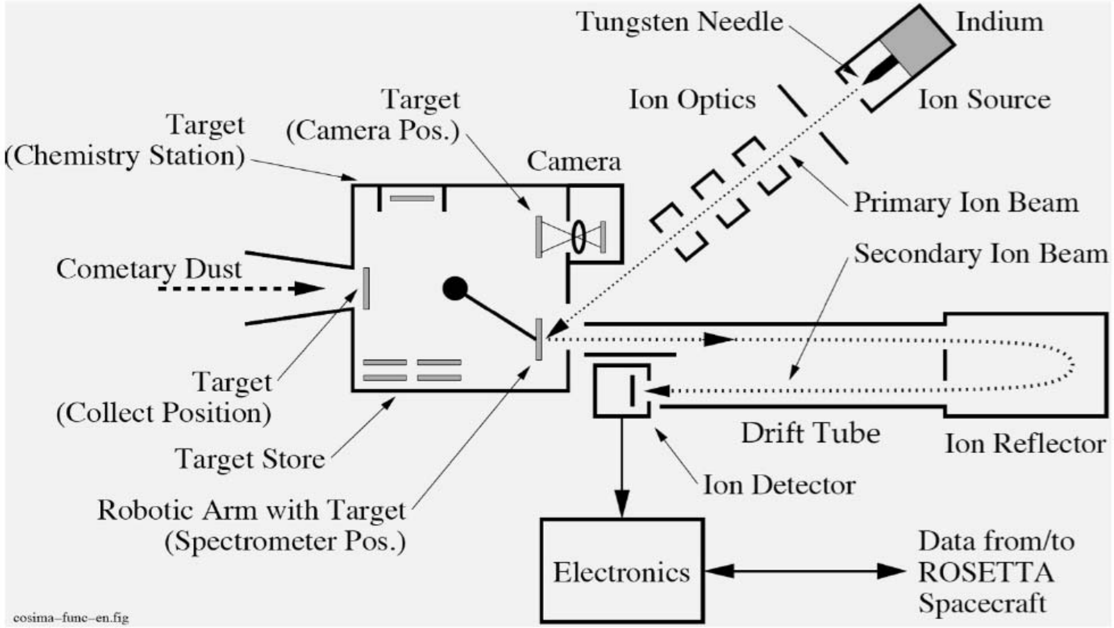

Figure 2: Diagram of the Cosima flight model. Cosima is a time of flight secondary ion mass spectrometer with a resolution mass resolution of about 1:1400 at 100u.

Method

Different crushed meteorite samples were arranged on a target plate and placed in the Cosima reference model (Figure 3). Hundreds of spectra were taken of these samples.

The resulting spectra are initially calibrated by the operational software pipeline. To facilitate the planned covariance/correlation analysis, the spectra are additionally rebinned to be as good aligned with each other as possible.

Covariances or Correlations between different mass numbers / time of flight measurements are calculated in the following way:
The spectra of the different samples are treated separately. For each sample a correlation matrix S is calculated in which each element s_{ij} corresponds to the Pearson correlation coefficient between time bins i and j. In this work we used the mass range between 1 u and 200 u for the correlation matrix.

That are round about 22000 time bins, leading to a matrix of about 484x106 elements. Depending on the number of spectra, this is a time consuming computation for which we developed a parallel Fortran code.

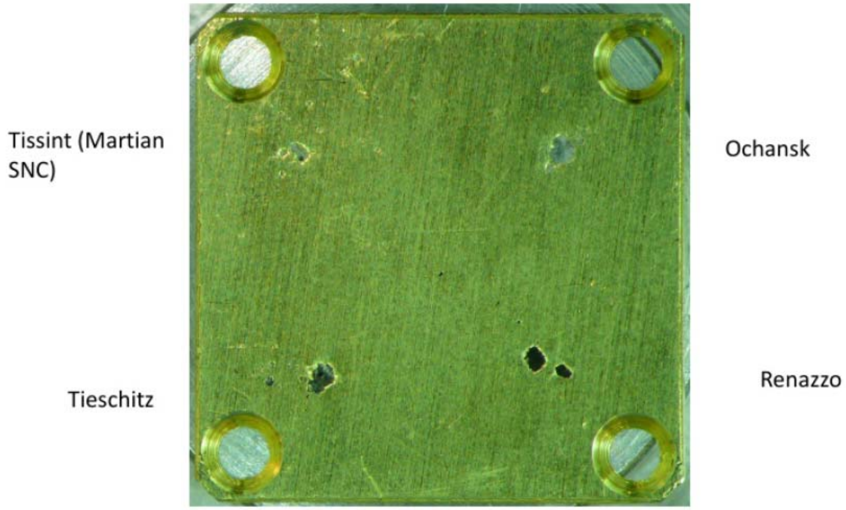

Figure 3: Gold target plate with four meteorite samples.

Results

Figure 4 shows parts of the correlation matrices for the four meteorite samples. Only a small mass range is shown here to make the high resolution visible.

Figure 5 shows the sums of the spectra for each sample in the same mass range.

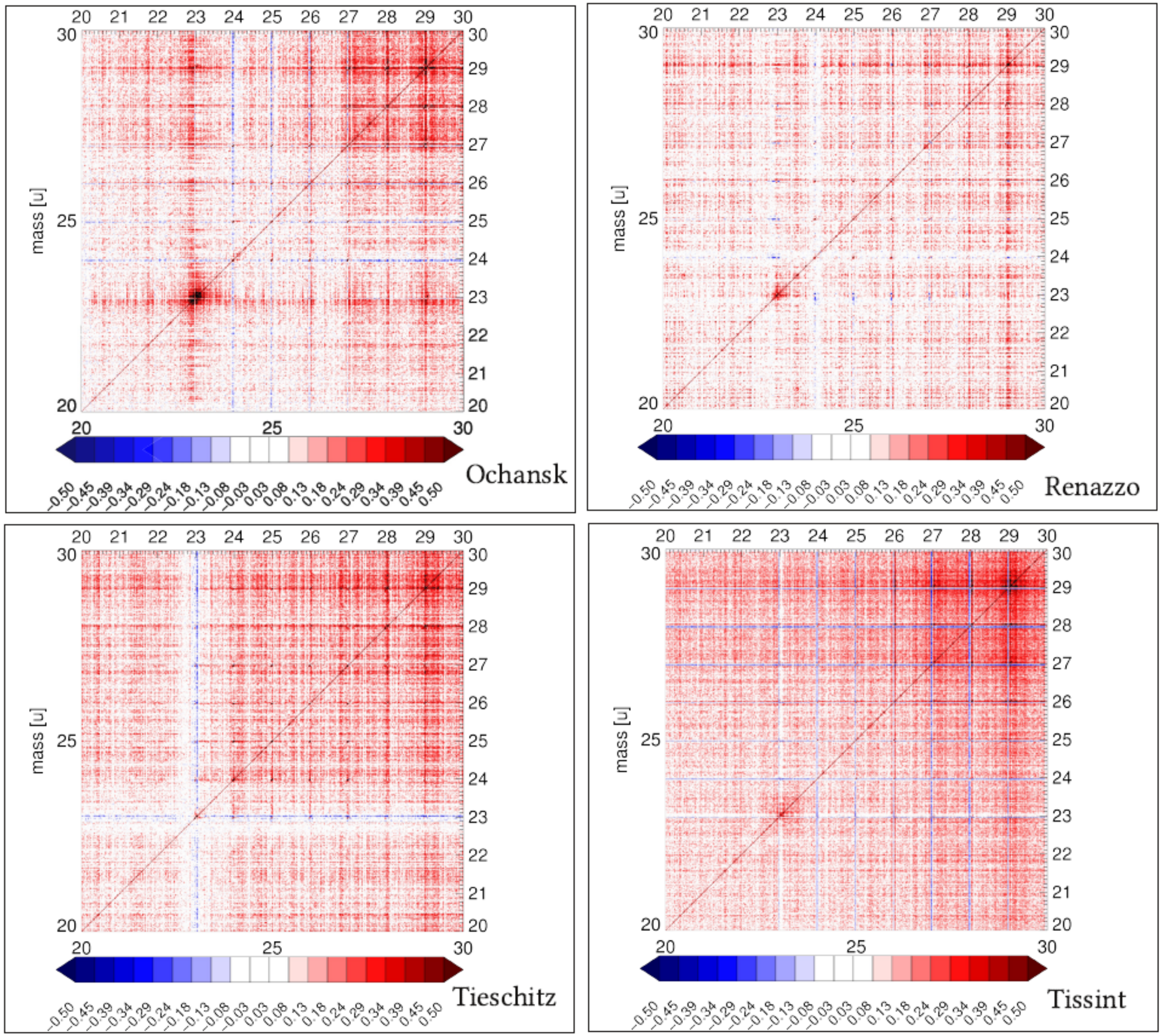

Figure 4: Correlation plot for four meteorite samples: Ochansk, Renazzo, Tissint, and Tieschitz, in the range of 20 to 30 u. Red shows correlation while blue shows anti-correlation. Since the actual peaks are very narrow (see Fig. 6), the plots are dominated by the mostly positive correlation from chemical noise.

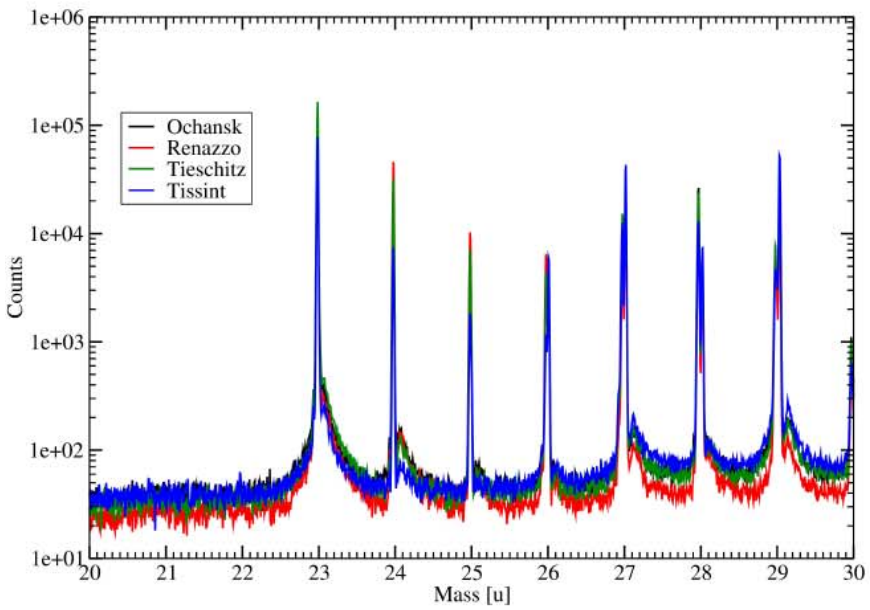

Figure 5: Cumulative spectra for each of the samples in the mass range from 20 to 30 u.

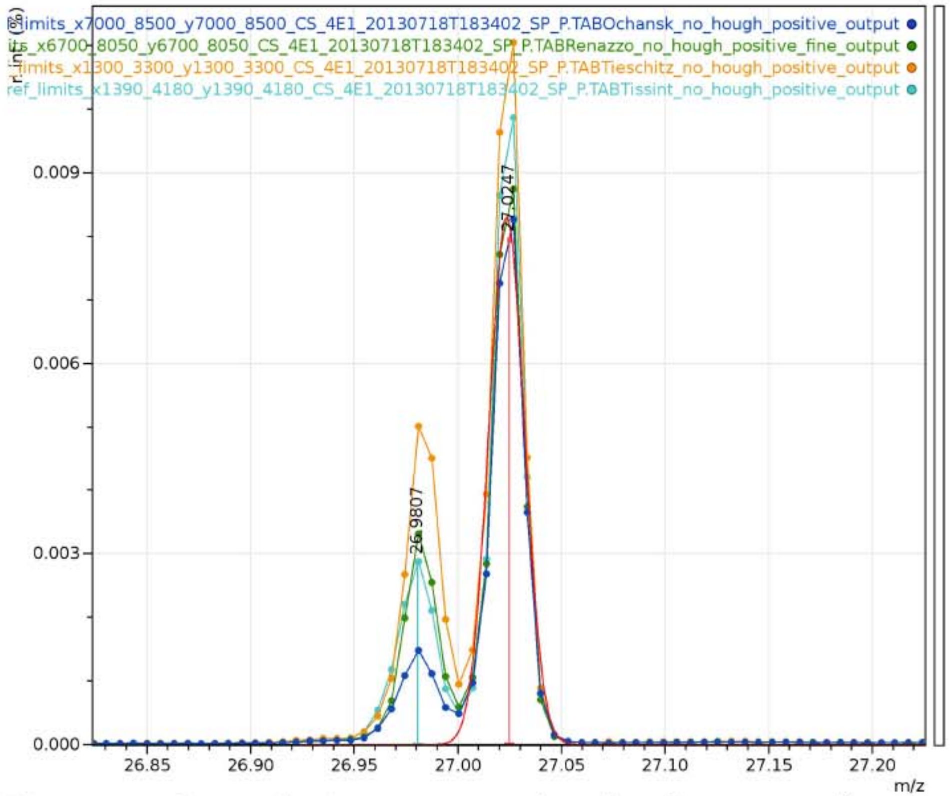

Figure 6: Cumulative spectra for the four samples at mass 27. The spectra have been recalibtrated using the free program mmass [4]. The mineral and the organic peaks are clearly separated. All spectra are normalized. The red curve shows a artificial C_2H_3 peak fitted to the observation of the Ochansk sample.

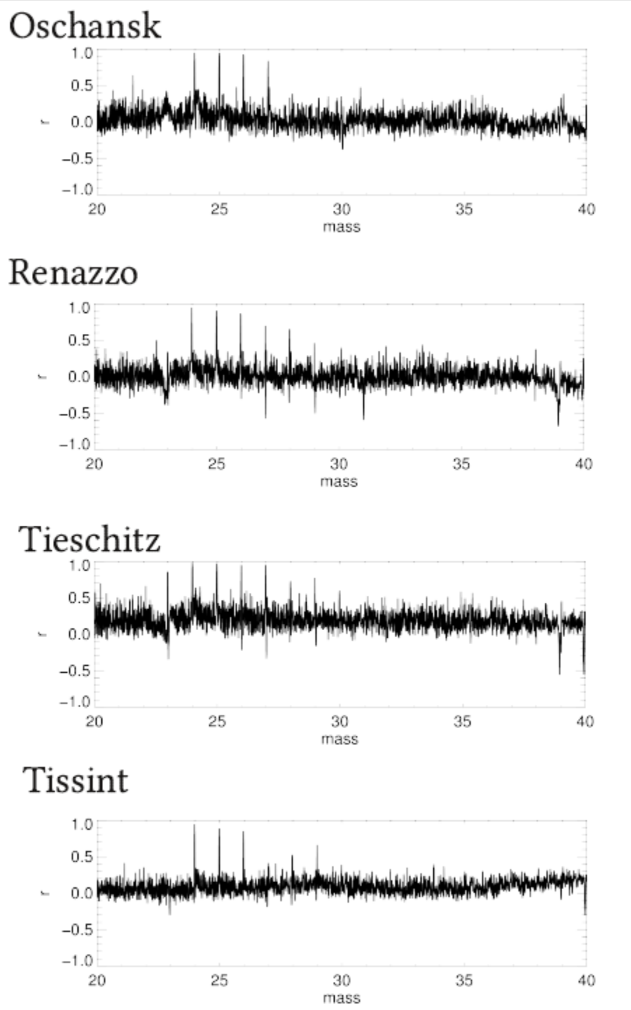

Figure 7: Correlation plots for ^{24}Mg.

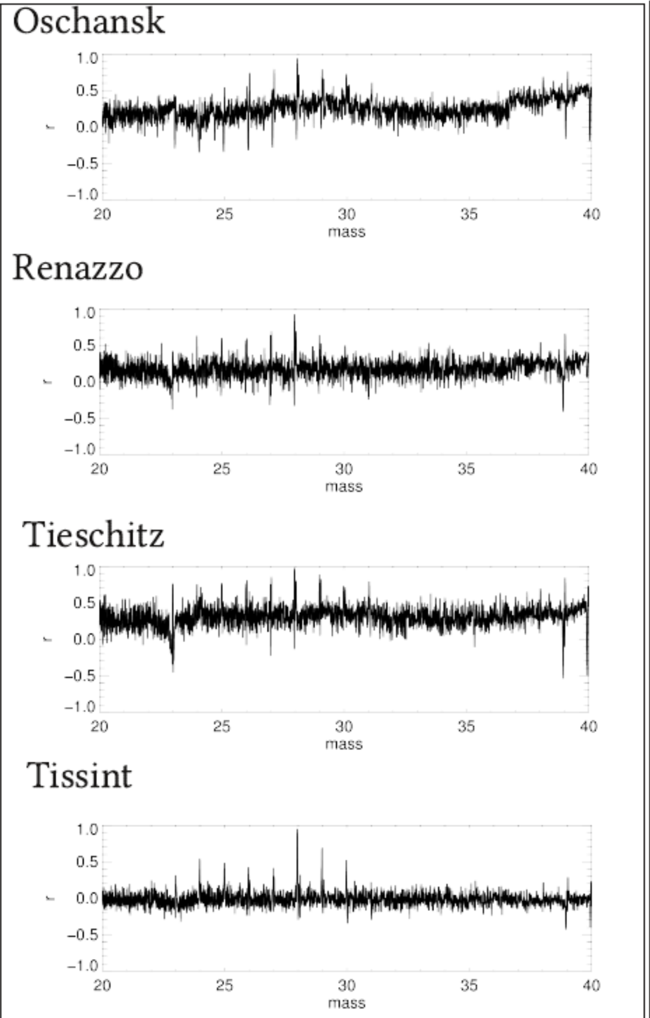

Figure 8: Correlation plots for ^{28}Si.

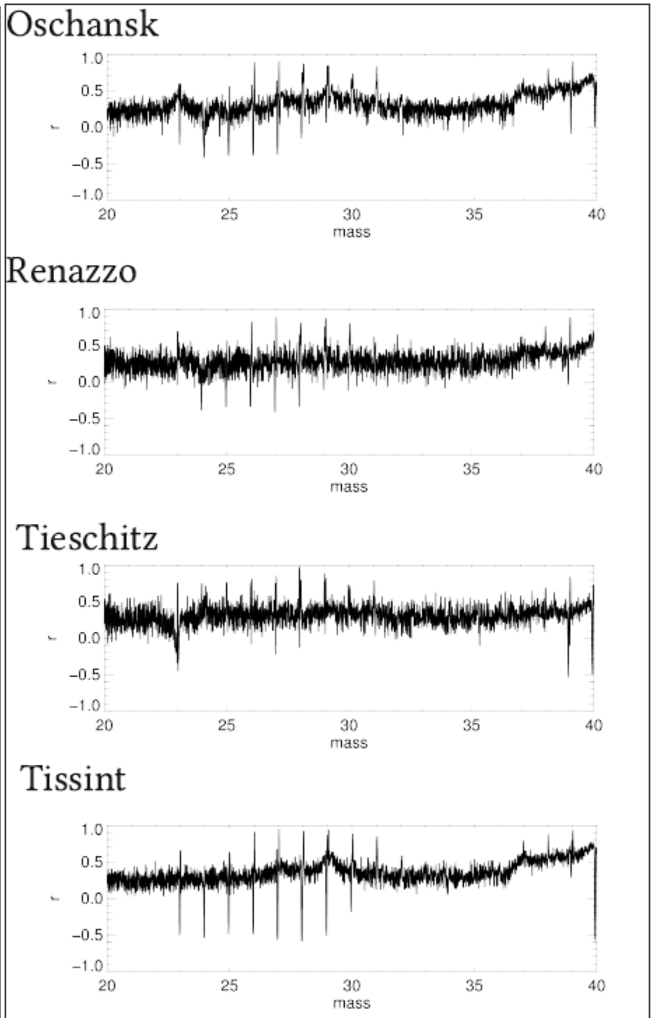

Figure 9: Correlation plots for C_2H_3.

Conclusions

Our correlation results show a clear separation between the inorganic (e.g. ^{24}Mg, ^{28}Si) and organic peaks. There is low correlation between the organic and the inorganic peak intensities, some show an anti-correlation.

All four samples show distinct patterns in the correlation matrices as well as in the single correlation plots.

This encourages the further investigations into correlations as a means to classify cometary samples within the references of meteoritic samples probed in the laboratory.

References

[1] Kissel J. et al. (2007) Space Sci Rev, 128, 823. 138, 243.
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[3] Varmuza, K. et al., (2011) Anal. Chim. Acta 705, 48–55.
[4] mmass http://www.mmass.org

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