Elemental surface composition of comet 67P grains (Rosetta) and of carbonaceous chondrite meteorites - characterized by multivariate mass spectral data (COSIMA)

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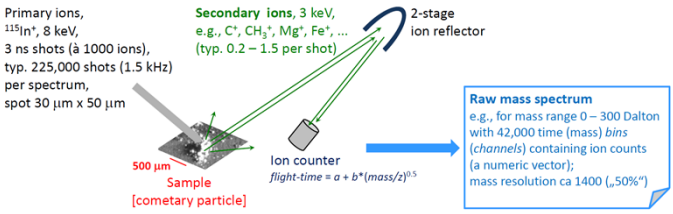
- **COSIMA** [1] was operated on-board of spacecraft **Rosetta**; it collected ca. 35,000 **cometary dust particles,** imaged them [2], and measured ca 34,000 mass spectra [3] on ca. 400 particles.
- **Meteorite samples** [4] have been used as references, analyzed with a laboratory twin instrument of COSIMA.
- Selected mass spectra have been evaluated in this work by **multivariate data analysis** (chemometrics [5]) to characterize the elemental and chemical composition.

Scheme of the mass spectrometer COSIMA

Surface analysis by secondary ion mass spectrometry (SIMS)
+ time-of-flight (TOF) mass separation of secondary ions



Elements (inorganics)

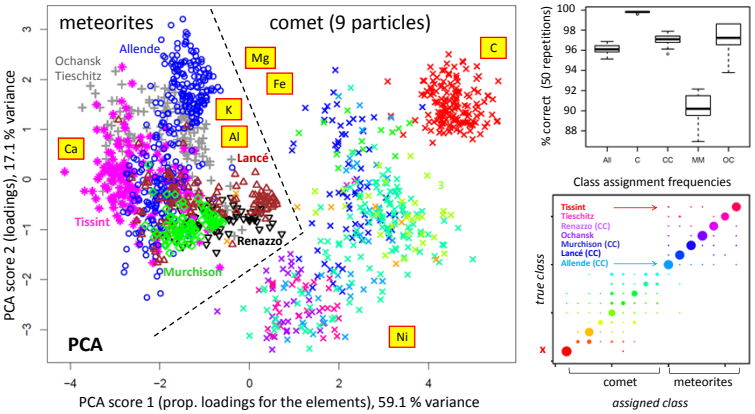
Aim. Comparison of patterns with relative element concentrations in cometary particles (**C**) and in carbonaceous chondrites (**CC**); with ordinary chondrites (**OC**) and a Martian meteorite (**MM**) as references.

Data

- COSIMA spectra: 509 from nine cometary particles; 619 from CC's (Allende, Lancé, Murchison, Renazzo); 145 from OC's (Ochansk, Tieschitz); 153 from MM (Tissint); total **1426 objects (cases)**.
- Counts of ***positive ions*** for C, Mg, Al, K, Ca, Fe, Ni; ***centered log-ratio transformed*** (compositional data [5]), giving **7 variables**.

Methods

- Exploratory data analysis by principal component analysis (**PCA**) [5]; biplot with scores and loadings.
- Classification by k-nearest neighbor method (**KNN**), combined with repeated double cross validation (**rdCV** [6]), estimating the variability of % correct assignments for test set objects (box plots).
- Software in R [7].



Results (based on used relative element concentrations and the used samples; details not presented here)

- Cometary particle surfaces are clearly different from the meteorites (CC, OC, MM).
- Cometary particles show higher carbon contents than the CC meteorites.
- Cometary particles (and meteorite grains) show varying heterogeneities.

CHNO compounds (organics)

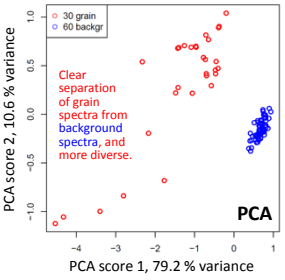
Aim. Search for secondary ions containing the elements C, H, N, O in COSIMA mass spectra measured at the surface of a cometary particle.

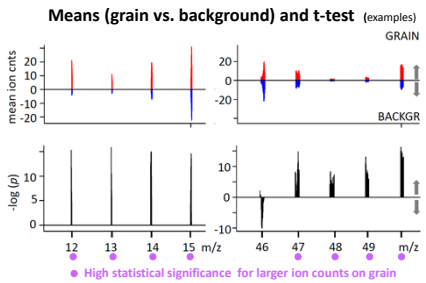
Data

- COSIMA spectra: $n1 = 30$ measured at a cometary particle (grain), $n2 = 60$ at Au background (substrate).
- Counts of positive ions at 665 mass bins, covering all 322 possible ion formulae with C, H, N, O in mass range 12 to 72. Mass intervals = $m \pm 1.5$ sd; m = theor. mass; sd = stand. dev. of Gauss peak (= $m/(2.36*R)$); R = mass resolution $m/\Delta m$ (50% peak height) = 1000.
- Ion counts (variables) normalized to sum=100.

Methods

- Exploratory data analysis by principal component analysis (**PCA**) [5].
- Comparison of the **means** for grain spectra and background spectra (each variable separately).
- Statistical **t-test** for zero hypothesis "data from grain and background from the same population". Evaluation by **-log(*p*)** = high for significant diffferences of the classes. Software in R [7].





- Ions potentially from the surface of the cometary grain: m/z {theor. ions} (**selection**, *guess*)
  12 {$\mathbf{C^+}$}; 13 {$\mathbf{CH^+}$}; 14 {$\mathbf{CH_2^+}$, N^+}; 15 {$\mathbf{CH_3^+}$, NH^+}; 24 {$\mathbf{C_2^+}$}; 25 {$\mathbf{C_2H^+}$}; 37 {$\mathbf{C_3H^+}$}; **. . .**
  47 {7 formulae CHNO (e.g., $CH_3O_2^+$, $C_2H_7O^+$, $CH_7N_2^+$, CH_5NO^+) and 3 formulae with Si (e.g., $SiOH_3^+$); . . .
- Ions, probably NOT from the cometary grain: $C_3H_{5-9}^+$, $C_4H_{7-9}^+$, $C_5H_{7-12}^+$

Results (based on used data selection and treatment; details not presented here)

- The cometary particle surface contains *CHNO* compounds (high statistical significance).
- No information about distinct organic substance classes in the cometary particle; complex mixture and/or high molecular weight structures [8] suggested.

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Dust grains have been collected near the comet 67P/Churyumov–Gerasimenko by the time-of-flight secondary ion mass spectrometer (TOF-SIMS) COSIMA on board of the Rosetta spacecraft. The measured mass spectra contain information about the inorganic and organic composition of the surface of the grains. For a comparison of this cometary material with carbonaceous chondrite meteorites, a twin laboratory instrument of COSIMA has been used to obtain mass spectra from grain surfaces of the meteorites Allende, Lancé, Murchison and Renazzo. Multivariate data analyses, based on signals from selected ions, indicate similarities of the chemical composition of the surfaces of different sample groups, as well as the heterogeneity of the grains.

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