Extraterrestrial material from a comet and from meteorites - analyzed by TOF-SIMS and data evaluated by machine learning approaches

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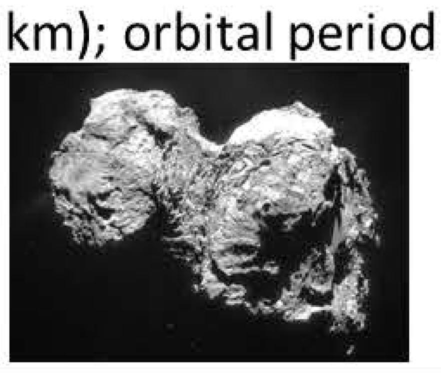
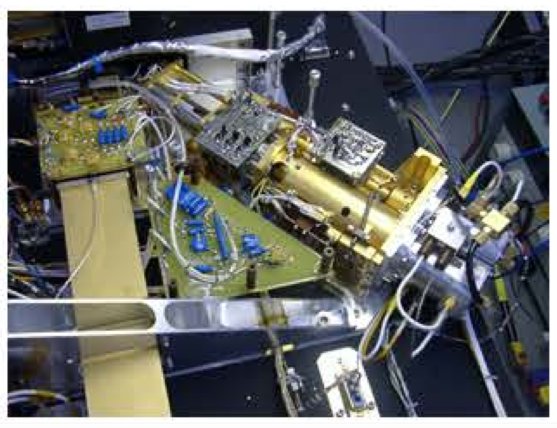
Comet. *Churyumov-Gerasimenko* code *67P*; size 4 x 3.5 x 3.5 km; density 0.533 g/cm³; distance from sun 1.24 – 5.68 AU (1 AU = astronomical unit ~150 000 000 km); orbital period 6.44 yr.

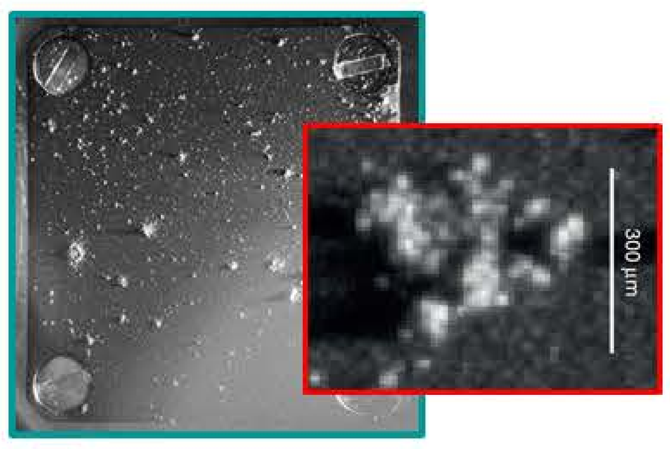


Rosetta. Space mission by ESA (European Space Agency); launch 2 Mar 2004; *near* comet 6 Aug 2014; turned off 30 Sep 2016.

COSIMA. Instrument onboard of Rosetta; collection of dust particles, imaging and analyzing by TOF-SIMS (time-of-flight secondary ion mass spectrometry) [1, 2].



TOF-SIMS. Prim. ions In^+, 8 keV; spot ~ 40 μm; inorganic/organic ions separated up to m/z ~100.



□ Gold target 1 x 1 cm with cometary particles, 50 – 700 μm diameter.
□ ~300 μm particle [3]

Meteorite samples

Carbon-rich meteorites (carbonaceous chondrites, CC) are sometimes considered to have a similar composition as comets. CC samples have been provided by the Natural History Museum Vienna [8].

Data evaluation

A typical data set in this work consists of matrices $\boldsymbol{X}(n \times m)$ and $\boldsymbol{Y}(n \times q)$ for n objects (spectra), m variables (features derived from TOF-SIMS data, ion abundances), and q sample classes. Methods applied from machine learning (multivariate statistics, chemometrics) are PCA, KNN classification, PLS discriminant classification, random forest classification, and others [8].

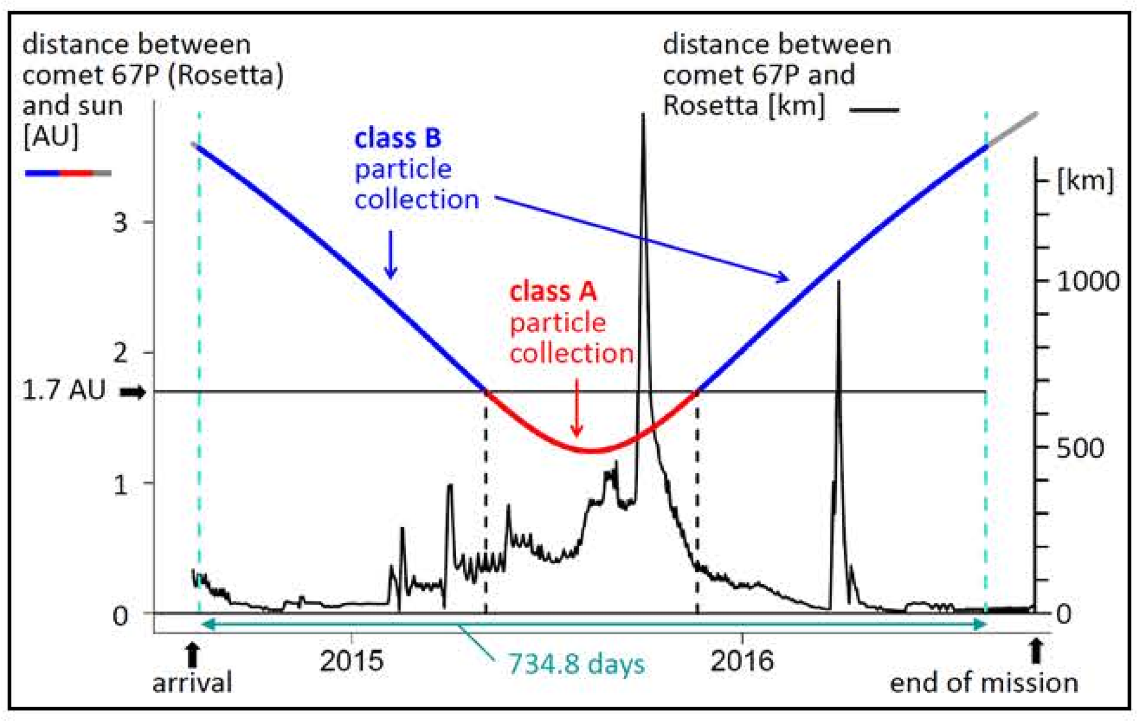
Composition of cometary dust collected near and far the sun

n = 2863 TOF-SIMS spectra measured at 256 particles

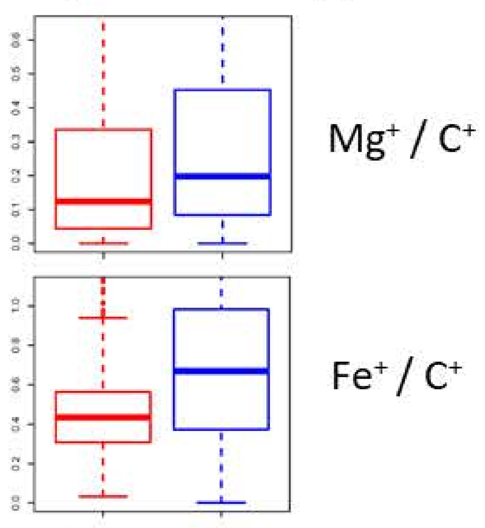
n_1 = 1459 in class A: collection at ≤1.7 AU (*near sun, warmer*)

n_2 = 1404 in class B: collection at >1.7 AU (*far from sun, cooler*)

m = 9 variables: ion counts for C^+, CH^+, CH_2^+, CH_3^+, Mg^+, $C_2H_3^+$, $C_3H_3^+$, $C_3H_4^+$, Fe^+, [4], normalized to sum 100 or transformed as compositional data by *centered log-ratios (clr)* [5].



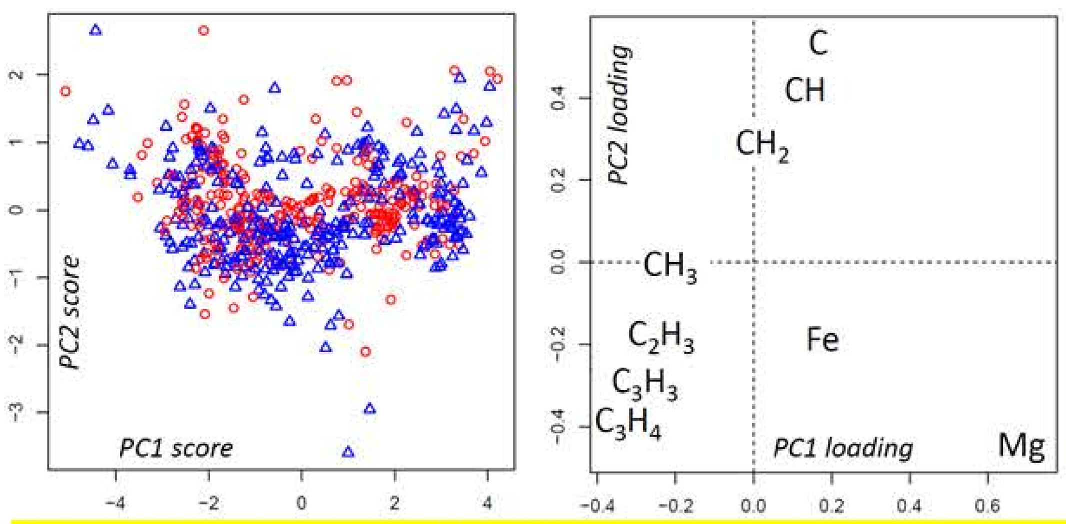
Uni/bi-variate approach



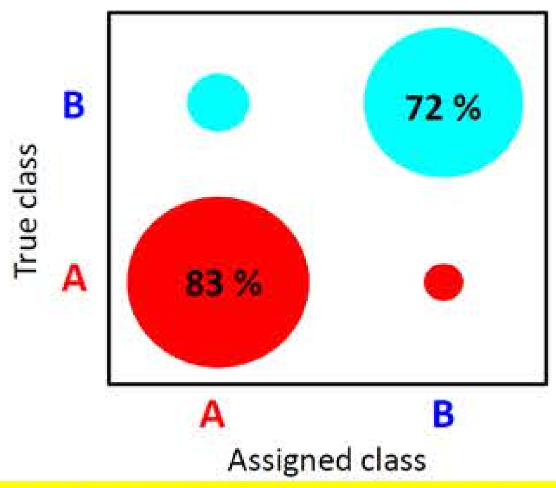
Tendency: enhanced C^+ in particles from *warmer* area.

Multivariate approach

PCA. n_1 = 300; n_2 = 300 (randomly); clr transformed. Variances of PC1, 2: 82.3, 10.9 %



KNN. All data; optimum k = 3 estimated by repeated double cross validation, rdCV [7].



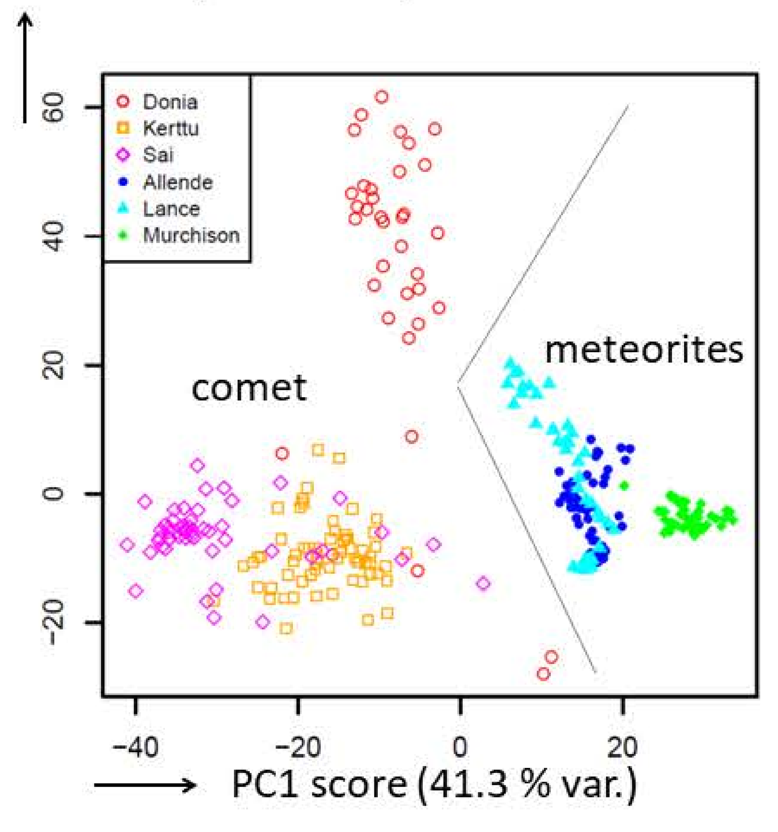
Clear separation of particles from *warmer* and *cooler* areas. Particles collected in the first part of the mission (*cool*) are from a dust coat that is removed near the sun. Near sun (*warm*) fresh material from the comet is measured with enhanced carbonaceous matter [1,5].

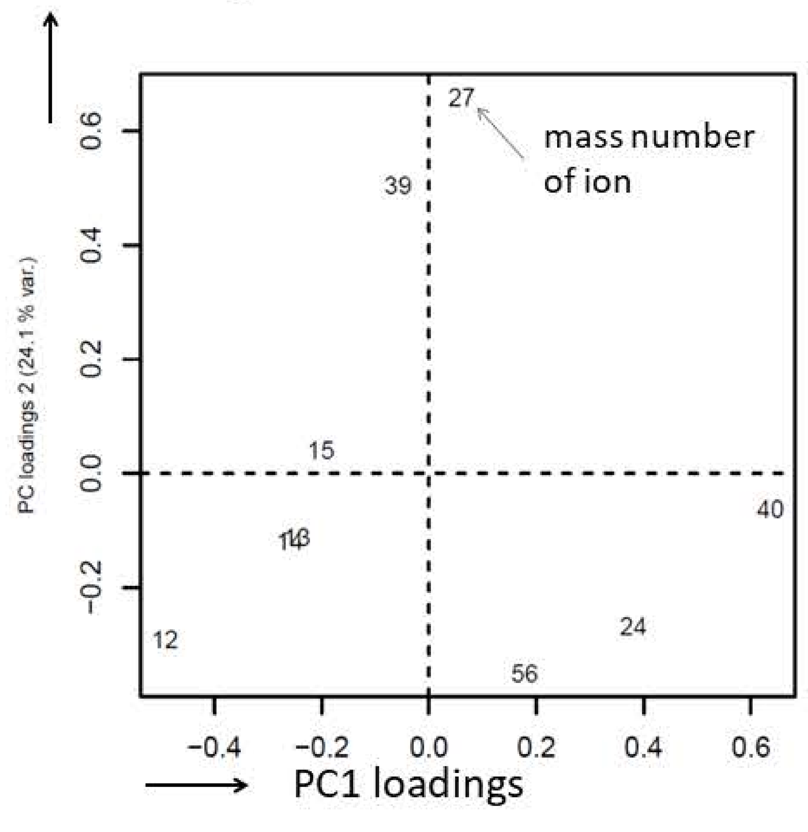
Cometary dust compared with carbon-rich meteorites

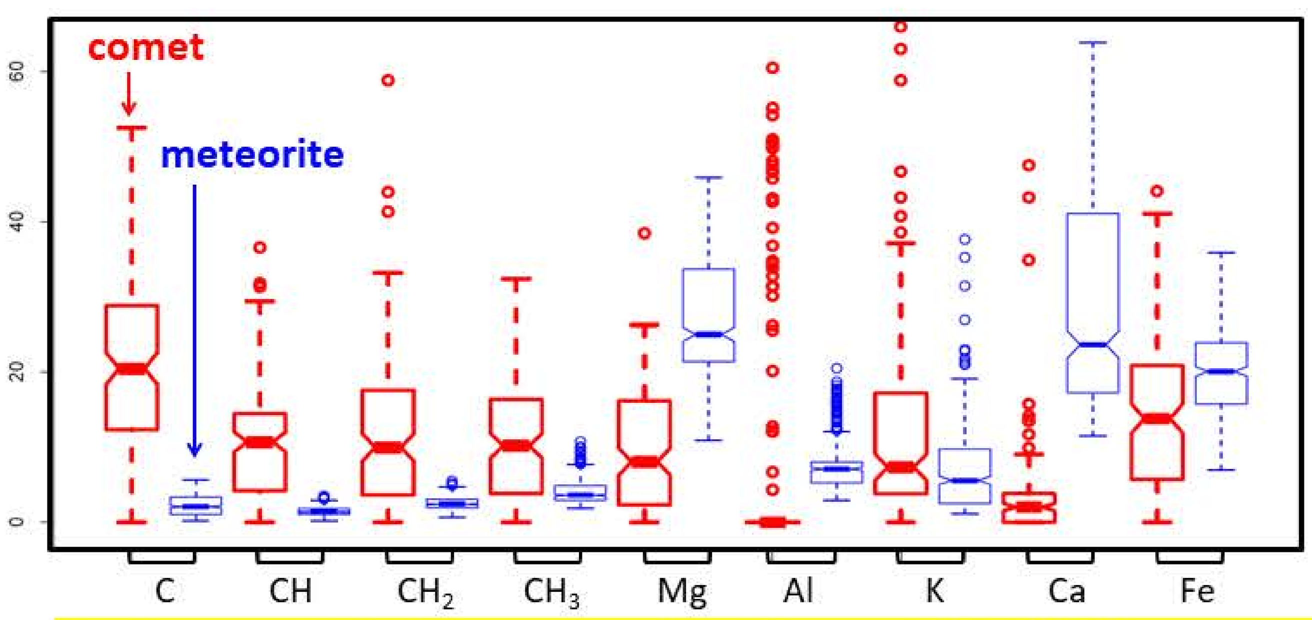
n = 301 spectra; 50 from each of the 3 meteorites Allende, Lancé and Murchison, and 151 from 3 cometary particles (Donia, Kerttu, Sai)

m = 9 variables: ion counts for C^+, CH^+, CH_2^+, CH_3^+, Mg^+, Al^+, K^+, Ca^+, Fe^+, (organics and inorganics), normalized to sum 100.

PCA







Univariate distributions of ion abundances

sum 100
n = 591

Carbon-containing ions are prominent in comet data [7,8].
Ca^+ and Mg^+ are more abundant in meteorites than in the comet particles.
The comet composition data are more diverse than the meteorite data.

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[2] Kissel J. et al.: *Space Sci. Rev.*, **128**, 823 (2007)
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[5] Filzmoser P. et al.: Applied compositional data analysis, Springer Nature (2018)
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[7] Stenzel O.J. et al.: *MNRAS*, **469**, Suppl_2, S492-S505 (2017)
[8] Varmuza K.: project website www.lcm.tuwien.ac.at/comecs/

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