

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

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Time-of-flight secondary ion mass spectrometry (TOF-SIMS) has been applied (a) to characterize the composition of cometary dust particles in situ near a comet (ESA mission Rosetta, onboard instrument COSIMA), and (b) to meteorite samples by a laboratory instrument (a twin of COSIMA) [1, 2]. The obtained multivariate data are relative abundances of secondary ions, containing information about the inorganic and organic composition of the analyzed material. Various chemometric methods (machine learning) supported the evaluation and comparison of the chemical analytical measurements. For two sub projects selected results are presented.

(1) The composition of cometary particles (typical diameter 50 - 800  $\mu\text{m}$ ) is different for sampling "near" the sun (1.24 - 1.7 AU) and "far" the sun (1.7 - 3.8 AU). The content of carbon-containing (organic) substances is enhanced in near-sun samples [3]. Note, the orbit of the comet is elliptic (1.24 - 5.8 AU distance to sun; AU stands for astronomical unit equal to 150 million km, the mean distance between earth and sun).

(2) The cometary samples show higher relative abundances of the secondary ions  $\text{C}^+$  and  $\text{CH}_{1-3}^+$  than carbon-rich meteorites (carbonaceous chondrites). In multivariate evaluations the cometary samples and these meteorites exhibit clearly separated clusters, for instance demonstrated in PCA (principal component analysis) score plots.

[1] Kissel J. et al.: *Space Science Reviews* **128**, 823-867 (2007)

[2] Fray N. et al.: *Nature* **528**, 72-74 (2016)

[3] Varmuza K. et al.: *J. Chemometrics*, **2020**, e3218, 1-8 (2020)

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