

ICP-MS of meteorite samples

Chemometric evaluation of diversity and discrimination

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- The surface of meteorite particles is characterized by **Laser Ablation - Inductively Coupled Plasma - Mass Spectrometry (LA-ICP-MS)**.
- The obtained relative elemental compositions are evaluated by multivariate data analysis.

Meteorite samples

Type	Name (number of spectra)	Total
Carbonaceous chondrite (CC)	Allende (182), Lancé (273), Murchison (288), Renazzo (555)	1298
Ordinary chondrite (OC)	Chelyabinsk (293), Mocs (72), Ochansk (384), Pultusk (32), Tieschitz (940)	1721
Planetary material	Moon (281), Mars (Tissint, 783), Vesta (asteroid, 289)	1353
Summary: 12 meteorite classes (3 groups)	Spectra	4371

LA-ICP-MS

Instrument: Thermo Fisher ICAP Q, with ESI NWR 213

Laser: Nd:YAG, $\lambda = 213$ nm (1064 nm quintupled),
fluence 8.8 J/cm² ($\pm 70\%$), spot 80 μ m diameter, scan speed 5 μ m/s

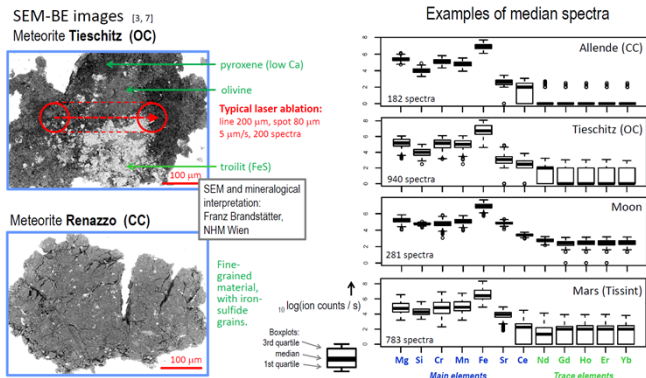
MS: Quadrupole (dwell time 50 μ s)

12 ion abundances (counts/s): ²⁵⁺²⁶Mg, ²⁹Si, ⁵²Cr, ⁵⁵Mn, ⁵⁶Fe, ⁸⁸Sr, ¹⁴⁰Ce,
¹⁴⁴Nd, ¹⁶⁰Gd, ¹⁶⁵Ho, ¹⁶⁶Er, ¹⁷⁴Yb

Multivariate data: X (4371 $\times$ 12) ion counts; y (1... 4371) class codes [1]

Software: R (Import of experimental ICP-MS data [2], chemometrics [1])

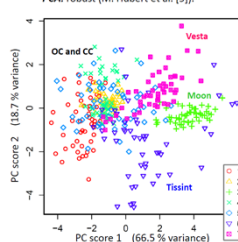
Spectral data



Exploration (PCA)

Principal component analysis

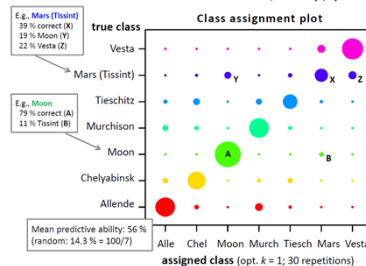
Data: 7 classes (Allende, Chelyabinsk, Moon, Murchison, Tieschitz, Tissint (Mars), Vesta). From each class 50 randomly selected spectra; $n = 350$; $m = 12$ variables.
Transformation: centered-log-ratio (clr) [4].
PCA: robust (M. Hubert et al. [5]).



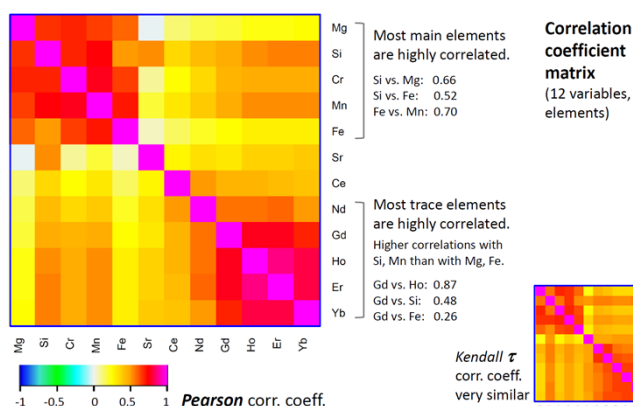
Discrimination (KNN)

k-nearest neighbor classification

Data: 7 classes as for PCA (see left). From each class 150 randomly selected spectra; $n = 1050$; $m = 12$ variables.
Transformation: constant row sum 100.
KNN: with rdcv evaluation, $k = 1-10$ [1, 6].



Correlation

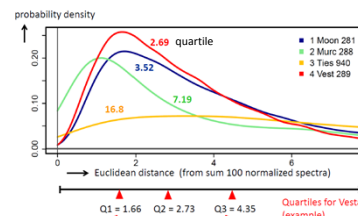


Spectral similarity

Aim: Characterizing the similarity of ICP mass spectra measured on grains from a particular meteorite class.

Similarity (dissimilarity) of 2 spectra
○ Euclidean distance (used here), d
○ Based on correlation coefficient

Method: Calculate the Euclidean distances, d , between all pairs of spectra (for a given class). The distribution of d characterizes the diversity of the spectra. A numerical measure is e.g., the IQR (interquartile distance) of d .



Summary

- LA-ICP-MS is a versatile technique for the determination of relative elemental compositions of meteorites.
- Simple sample preparation; destructive.
- Multivariate data analysis of LA-ICP-MS data may support the discrimination of meteorite classes.
- The work is related to the evaluation of TOF-SIMS data from cometary particles in the Rosetta/COSIMA project [7].