

Oral presentation

## Classification and characterization of materials – from archaeometry to comets

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Materials of various origins and produced for various applications have a complex composition and can be sufficiently characterized only by a multitude of data – often spectroscopic data or the concentrations of several components in the material. Typically, the relationships between measured data and interesting properties or class memberships of the materials cannot be described by theory but require empirical models, that have to be derived from data originating from materials with known measurements and properties.

Methods from multivariate data analysis are powerful tools for analyzing such data and for creating mathematical models; this is the essential part of today's chemometrics [1]. A user-oriented overview of some widely applied methods in exploratory data analysis, multivariate classification, and multivariate calibration will be given – avoiding any detailed mathematics. Basic ideas, such as the optimum complexity of models, selection of an effective subset of the measurements, as well as a realistic estimation of the performance of calibration models will be discussed.

A number of examples illustrate the use of multivariate data analysis in chemistry: The origin of an organic material found in traces on a Neolithic statuette is identified from GC/MS data. The heating values of biomass materials are estimated from the elemental compositions and from IR data. Organic and mineral reference materials, that are relevant for future mass spectroscopic measurements near a comet, are classified.

### References

1. Varmuza K, Filzmoser P: **Introduction to multivariate statistical analysis in chemometrics**. CRC Press, Boca Raton, FL, USA; 2009 in press.