Comprehensive IR data analysis methods for the study of oil paint degradation processes

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Abstract:

Oil paintings present an interesting challenge to analytical chemistry, with samples that are insoluble, highly heterogeneous and very precious. Infrared microscopy is a common technique to study oil paint, and it is usually straightforward to identify pigments, binders or degradation products that dominate a given set of spectra. However, an IR microscopy dataset can contain much more information about, for instance, compounds present in low concentration or subtle changes in molecular structure, even when spectra are very congested and absorption bands overlap. The large amount of data collected in a typical IR hyperspectral datacube is ideal for the application of automated analysis algorithms that can reveal the chemical diversity in a sample and support a detailed interpretation of spectra.

In this talk, a general outline will be given for a comprehensive data analysis approach, including PCA-type methods, peak position analysis and constrained band fitting, in an effort to obtain quantitative information on the distribution of chemical species. To illustrate the methods, we will focus on oil paint samples that exhibit zinc soap formation, a common problem in modern oil paintings. Using our methods, it iss possible to disentangle at least four different zinc carboxylate species, resolve their structures and map their spatial distribution. The results give important new insights in the chemical mechanisms that cause zinc soap formation and oil paint ageing in general.