Comprehensive structural analysis of soot samples with different OC content by means of HRTEM, FTIR spectroscopy and Raman microspectroscopy

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Aerosols are of importance for the climate, the environment and the human health. One key component in the atmospheric aerosols are carbonaceous materials, which are mainly of anthropogenic origin and formed by the incomplete combustion of fossil fuels or biomass burning.

The characterization of carbonaceous aerosols or soot, is often performed by thermo-optical methods to determine the content of organic carbon (OC) and elemental carbon (EC). Although these methods are commonly used, there are soot properties (e.g. reactivity, hydrophilicity) that cannot be explained by the EC/OC ratio. Furthermore, it is not clear whether the OC content in the soot is related to differences in the soot structure.

Therefore, we performed a comprehensive study on the structure of soot generated by a CAST burner with different propane-to-air ratios. We applied thermo-optical analysis (Sunset Lab, IMPROVE protocol, (Chow *et al.* 1993)) to determine the EC/OC ratio, transmission electron microscopy (TEM) and high-resolution transmission electron microscopy (HRTEM) to reveal the micro- and nanostructure of soot, FTIR spectroscopy to gain information on the organic compounds and Raman microspectroscopy (RM) to characterize the soot composition and structure.

The FTIR analysis of the soot samples with different OC content (4%, 47% and 87% OC) revealed the organic composition of the samples, showing increased aromatic vibrations for samples with higher OC content. RM, which is based on the effect of inelastic light scattering provides the information on the soot structure (including disordered graphitic and amorphous carbon) (Ivleva *et al.* 2007, Parent *et al*. 2016). Thus, the RM-results of the soot samples gave an increased fluorescence background and an additional shoulder in the spectrum from organic compounds (e.g., C–O str.) with increasing OC content. According to the peak ratio of the Raman soot peaks and in agreement with HRTEM-analysis, the nanostructural order was high for the soot with 4% of OC and low for the soot with 87% of OC (Ess *et al.* submitted).

RM results in combination with IR, TEM and HRTEM data should help us to get better insight into complex composition and structure of soot samples, and improve the understanding of soot properties (e.g., reactivity and hygroscopicity), which vary significantly for soot samples with different OC content.

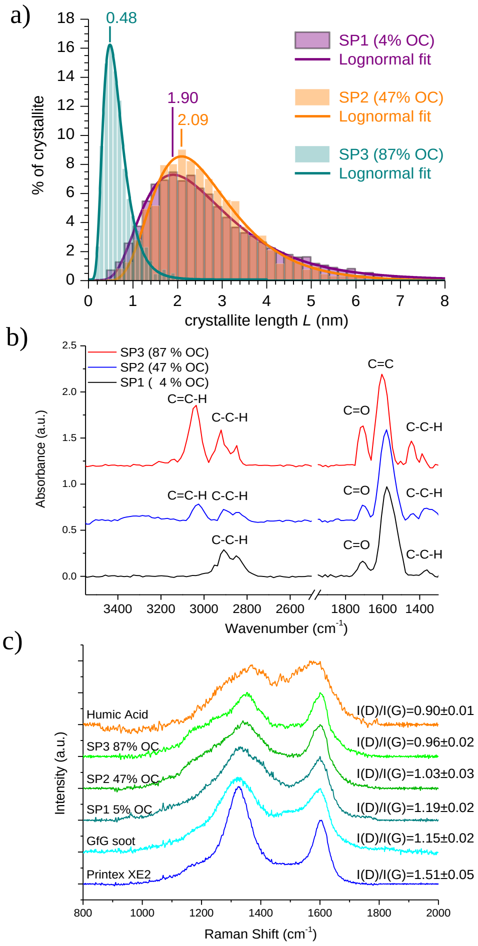

Figure 1. Crystallite size distribution obtained by HRTEM (a), FTIR (b) and Raman (c) spectra of soot with different OC content (Ess *et al.* submitted).

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