Online Proton-transfer-reaction and Resonance-enhanced multiphoton ionization mass spectrometry for monitoring the coffee roast process

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Coffee is one of the most traded commodities and is one of the most consumed beverages worldwide with an estimated coffee consumption of 4 kg per capita in Switzerland. Coffee, e.g. Arabica coffee (*Coffea arabica*) is harvested and processed in the origin countries to produce the green beans. The roasting process transforms then the green beans into roasted coffee and thereby producing a drinkable product. Coffee roasting itself is an extremely complex chemical and physical process leading to the formation of a large number of (semi)volatile organic aroma compounds. However, the dynamics and mechanisms of these formation processes are not completely understood and specific characteristics of the roast process such as the actual roast degree are often determined empirically or based on individual experience. Hence, on-line monitoring of the roasting process is important to understand the underlying chemical reactions and to ensure an optimum product. Direct mass spectrometry applying soft ionization techniques is a powerful method to study the roast process in real time. We have applied direct mass spectometry to coffee roasting in the form of proton-transfer-reaction mass spectrometry (PTR-MS) and photo-ionization time-of-flight mass spectrometry (PI-TOF-MS).[1]

On the one side we used PTR-ToF-MS, where we sample and analyse the roast gas and with it the produced volatile organic compounds (VOCs). This is an indirect method, which allows the real-time monitoring of the formation pattern of important coffee aroma compounds along the roasting process. By varying the time-temperature roasting parameters (roast degree and length of roasting process) as well as the coffee species and coffee origin reveals then changes in the coffee flavour formation: (i) different VOCs were formed differently while roasting the same type of coffee along the same time-temperature roasting profile, (ii) these formation pathways changed when changing the time-temperature roasting profile, and (iii) roasting different coffee origins led to different flavour formation pathways for the same VOCs. From a technical perspective, this study underlines the importance of taking into account the roasting parameters like flow of hot air for the different roaster configurations. A proper normalization of the VOC intensities with the flow parameters, pressures and temperatures is indispensable for a comparison of VOC formation between different roaster configurations.

A different way to detect VOCs can be carried out be resonance-enhanced multiphoton ionization time-of-flight mass spectrometry (REMPI-ToF-MS). Photo-ionization was employed to investigate more fundamental questions to examine chemistry and kinetics of VOC formation in individual single coffee beans.[2] The observed chemistry in single bean experiments reflects bulk roasting processes well, thus both approaches, PTR and PI, may be combined to improve the understanding of the chemical mechanisms during coffee roasting. This approach takes into account that the integrity of individual beans plays a decisive role for the formation of coffee flavour.

[1] Biasioli, F.; Yeretzian, C.; Gasperi, F.; M„rk, T. D., PTR-MS monitoring of VOCs and BVOCs in food science and technology. *Trends in Analytical Chemistry* **2011,** *30* (7), 968-977.
[2] Hertz-Schönemann, R.; Dorfner, R.; Yeretzian, C.; Streibel, T.; Zimmermann, R., On-line process monitoring of coffee roasting by resonant laser ionisation time-of-flight mass spectrometry: bridging the gap from industrial batch roasting to flavour formation inside an individual coffee bean. *Journal of Mass Spectrometry* **2013,** *48* (12), 1253-1265.