MO 3: Biomoleküle 2

Zeit: Montag 16:30–17:00 Raum: VMP 6 HS-F

MO 3.1 Mo 16:30 VMP 6 HS-F

Raman Spectroscopy as a Rapid Tool for the Determination of Free Fatty Acid in Extra Virgin Olive Oil — •Rasha Hassanein, Patrice Donfack, and Arnulf Materny — Jacobs university Bremen, Germany

Raman spectroscopy provides useful information about the molecular structure even in complex systems due to the fingerprint properties of the vibrational spectra. It has proven a potential analytical tool in food analysis, *e.g.* for oil authentication, classification, and in adulteration detection. In our research, we have demonstrated the potential of Raman spectroscopic with visible light (VIS) excitation for the determination of the free fatty acid (FFA) content of extra virgin olive oil in combination with multivariate analysis. To the best of our knowledge, none of the previous research works reported the use of VIS Raman for the FFA content measurement. However, this method offers many advantages; high sensitivity and high spectral resolution can be achieved in short time using a simple Raman setup. Another very important advantage is that the VIS excitation helps to resonantly excite (electronic resonance) vibrational bands of important constituents of oils such as carotenoid pigment molecules, which due to their low concentration cannot be detected using *e.g.* IR Raman techniques. In our approach, a model was constructed with partial least square regression in order to predict the FFA content in extra virgin olive oil based on the VIS Raman data. The regression results showed a strong correlation between FFA content and the presence of carotenoids.

MO 3.2 Mo 16:45 VMP 6 HS-F

Organic Molecules in Supercritical Fluids: Solubility and Shift of Phase Boundaries — •Adnan Sarfraz, Wolfgang Christen, and Klaus Rademann — Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Strasse 2, 12489 Berlin

The dissolution of organic molecules in supercritical fluids has manifold applications, e.g. in supercritical fluid chromatography and the formation of nano-sized particles. To facilitate the process of dissolution, co-solvents are employed frequently. The addition of co-solvents shifts the phase boundary of the mixture; in most cases this shift is estimated theoretically. The knowledge of the critical point of the mixture is important to fully utilize the solvating capabilities. Using a new setup we can determine the phase boundaries of pure and mixed substances experimentally. The basic idea is the increased scattering of light in the vicinity of the gas-liquid phase boundary. We report results on the shift of the critical point of ethylene on addition of ethanol. Furthermore, in a continuation of the previous work on mass spectrometric detection of nucleobases in expanded supercritical fluids, we report on the pressure dependence of their solubility in supercritical ethylene with ethanol as co-solvent.