Appendix A. Supplementary material

Mid-IR Dispersion Spectroscopy – A New Avenue for Liquid Phase Analysis

Alicja Dabrowska, Stefan Lindner, Andreas Schwaighofer*, and Bernhard Lendl*

Research Division of Environmental Analytics, Process Analytics and Sensors, Institute of Chemical Technologies and Analytics, Technische Universität Wien, Getreidemarkt 9/164-UPA, 1060 Vienna, Austria

DESCRIPTION OF CONTENTS:

Figure S1. Schematic representation of the experimental setup measuring in the absorption spectroscopy mode.

Figure S2. The dynamic range of the EC-QCL MZI setup operating outside of the quadrature point.

Figure S3. The modelled refractive index uncertainty for various laser sources with various laser linewidths employed in the current experimental setup.

Figure S4. Impact of the temperature fluctuation noise on the optical displacement measurement.

Figure S5. First derivative of the refractive index spectra recorded with the MZI setup in transmission (d=25 μ m) for 2.5-50% v/v of ethanol.



Figure S1. Schematic representation of the experimental setup measuring in the absorption spectroscopy mode. The beam transmitted via the first beam splitter is blocked by a beam shutter.

The refractive index spectrum can be alternatively obtained without the active movement of the piezo-mirror. It will be calculated directly out of the differential signal (I_{diff}) recorded by the two detectors:

$$\Delta n \approx \frac{\lambda}{2\pi} \cdot \frac{\sqrt{2}}{d} \arcsin(I_{diff}).$$
(S1)

In this case, due to the lack of active movement of the piezo-actuator to hold the quadrature point, the system operates along the interference slope (out-of-quadrature) in the so-called working region (see Figure 1 in the main manuscript). This type of acquisition, although decoupled from the performance of the used piezo-element is sufficient for analysis of optically thin samples, however faces a number of issues which limit the technique's stability, sensitivity, dynamic range and precision when strongly absorbing samples are measured (see Figure S2).



Figure S2. The calibration curve from the dispersion spectra of ethanol (0.5-50% v/v) in water acquired without active compensation to the quadrature point. It illustrates the dynamic range of the EC-QCL MZI setup operating outside of the quadrature point along with varying sensitivities.



Figure S3. Blue line shows the modelled refractive index uncertainty for various laser linewidths employed in the current experimental system calculated for the center wavelength of 10 μ m (1000 cm⁻¹). Black dot indicate the current level of refractive index measurement uncertainty for the presented setup employing a pulsed EC-QCL with linewidths of 12 GHz.



Figure S4. Impact of the temperature fluctuation noise on the optical displacement measurement. (A) Temperature readout at the position of the temperature cell with and without the housing compared with (B) the simultaneous displacement readout of the piezo-mirror while the interferometer is locked to the quadrature point at a single wavenumber (1100 cm^{-1}) .



Figure S5. First derivative of the refractive index spectra recorded with the MZI setup in transmission (d=25 μ m) for 2.5-50% v/v ethanol.