

Abstract

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Title of diploma thesis: Application of Raman spectrometry for analysis of selected mixtures

The identification and determination of methanol and ethanol using Raman spectroscopy was tested. For such tests two types of calibration standards were prepared. The volumes of analytes used were adjusted to get the final concentration of the alcohols corresponding to 40 volume %. In the first type of calibration varied amounts of methanol and ethanol were applied, in the second different amount of methanol was used.

Measurement was carried out using portable dispersive Raman spectrometer with laser with an excitation wavelength of 785 nm. The effect of the measurement conditions to linearity of the calibration obtained in the evaluation of the signal intensity and the area of the intense band in the spectrum were tested in detail. Measurement conditions included the integration time (1000 ms, 2500 ms, 5000 ms and 7500 ms), the laser intensity (100 and 75%) and temperature (laboratory and 4-8 °C). Calibration standards and samples were measured in glass vials.

To identify the analytes whole Raman spectrum was compared. To compare the linearity of the calibration using the partial least squares the calibration curves were evaluated by an area of selected intense band and its intensity. Linearity for all measurement conditions met only evaluation by band area. Following conditions were chosen for the determination of analytes: integration time of 5000 ms, 100% laser intensity and laboratory temperature.

The amount of ethanol was determined in seven tested spirits. The content of methanol and other impurities was not determined, none of the tested substances (ethyl acetate, isoamyl alcohol, isobutanol) was found in the spectrum.

The identification and determination of sugars (glucose, fructose) in syrups were tested too. Seven selected samples were analyzed, sugars were identified and determined. In the house-made cherry liqueur sugars were identified and ethanol determined.