

FRI-ONLINE-1-CT(R)-01

APPLICATION OF CHEMOMETRIC METHODS COUPLED WITH INFRARED SPECTROSCOPY FOR DETERMINATION OF ETHANOL IN PRESENCE OF METHANOL IN AQUEOUS SOLUTIONS¹

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Abstract: A fast and cost-effective method, based on Fourier Transformed mid-Infrared Spectroscopy measurement coupled with chemometric method was developed for determination of ethanol in aqueous solutions at room temperature and presence of methanol. In order to facilitate the calibration process, and to minimize the effects of peaks' overlapping, an appropriate preprocessing of the IR signals was performed. The calibration was performed using 43 samples, with accuracy enough high, so that this method can be used in routine determinations of ethanol. The model was also tested on a separate set of other 9 validation samples, where it showed great performance with R² of prediction >0.99. Consequently, the procedure can be used as a fast and reliable determination of ethanol in aqueous solutions containing methanol as a second alcohol. The method can therefore find application in different areas of the chemical and food industry, avoiding use of chemicals, consumables or expensive equipment as HPLC. In fact, this approach could be used in other applications where distinguishable signals in FTIR exist, as for example quality control in production of fuels, essential oils, biodiesel, drugs etc.

Keywords: Partial least squares, chemometric, FTIR, calibration, ethanol, methanol

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¹ Reports Awarded with "Best Paper" Crystal Prize - 59th Science Conference of Ruse University, Bulgaria, 2020, as a hard copy (ISBN 978-954-712-826-2) and on-line on the Conference Website

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