A quantitative analysis of liquid hydrocarbon mixtures on the basis of FT-Raman spectra registered under unstable conditions.

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Streszczenie

The impact of environmental and spectrometer parameters on the FT-Raman Partial Least Squares quantification of cyclohexane, isooctane, toluene and *p*-xylene mixtures was investigated. Expressing composition in terms of mass fraction instead of molar concentration simplified the analysis although it caused a slight increase of the relative standard error of prediction (RSEP) for testing samples. Incident laser power, position of the sample, aperture settings and other factors influenced noticeably the obtained results, unless samples were analysed using models based on spectra registered under the same circumstances. In the latter case the RSEP values of the order of 0.5–2% were found. Adjusting the spectrometer during sample set measurements resulted in an increase of the RSEP values up to 4.5%. The normalisation of spectra by the selected band intensity of 2-chlorophenol added to mixtures lowered these values at least by a factor of 2. Almost the same result could be obtained by applying one constituent of the sample as an internal standard. A similar pattern was observed when the experimental room temperature was not stable. The quantification of samples, in which spectra were registered when more than one spectrometer and/or environmental parameter was changing, on the basis of the model constructed for optimal conditions gave mean RSEP values reaching 14% when the unnormalised spectra were used. Application of normalised spectra usually resulted in reduction of these errors to 2–3% level.

Słowa kluczowe

FT Raman spectroscopy, Quantitative analysis, Hydrocarbon mixture