Multivariate estimation between mid and near-infrared spectra of hexafluoroisopropanol-water mixtures.

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Streszczenie

Multivariate regression based on partial least squares (PLS2) was applied to estimating one spectral dataset from another set having an intrinsic relationship with each other. An estimation was successfully carried out between mid-infrared (IR) spectra in the range of 2980 - 3800 cm^{-1} and that of near-infrared (NIR) spectra in the range of 6000 - 7500 cm^{-1} for hexafluoroisopropanol (HFIP)-water mixtures. The result demonstrates that, after building a suitable regression model, not only NIR spectra, but also well-resolved IR spectra of HFIP-water mixture can be estimated properly in this way. The use of IR and NIR spectroscopy together with PLS2 regression will not only alleviate laborious and costly measurements, but also open a way to provide easier assignments of generally weak and highly overlapped NIR spectral bands.

References (18)