Water-Methanol and Water-Acetonitrile Mixture Analysis using NIR Spectral Data and Iterative Target Transform Factor Analysis

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Water-methanol and water-acetonitrile mixtures are frequently used as HPLC solvent system and strong hydrogen bonding is well-known. But a detailed aspect of water-methanol and/or water-acetonitrile mixtures have not been shown with direct spectral evidence. Recently, near infrared spectroscopy and chemometric data refinery have been successfully combined in many applications. On the basis of factor analytical methods, the spectral features of water-methanol and water-acetonitrile mixtures were studied to reveal the detail of mixtures.

Water-methanol and water-acetonitrile mixtures were prepared with varying concentration of each constituent and near infrared spectral data were acquired in the range of 1100-2500nm with 2-nm interval. The data matrices were analysed with ITTFA(Iterative Target Transform Factor Analysis) algorithm implemented as MATLAB codes.

As a result, the concentration profiles of water, methanol and water-methanol complex were resolved and the spectra of water-methanol complexes were calculated, which cannot be acquired with pure complexes. A similar result was obtained with NIR spectral data of water-acetonitrile mixtures. Moreover, pure spectra of hydrogen-bonding complexes of water-methanol and water-acetonitrile can be computed, while any other usual physical methods cannot isolated those complexes for acquring pure component spectra.

Keywords: water-methanol mixtures, water-acetonitrile mixtures, ITTFA, NIR spectra