Quantitative Fourier transform infrared and principal component analysis of polyaniline-polyvinyl alcohol-chitosan hydrogels

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Abstract

A combined synchrotron radiation-based Fourier transform infrared (SR-FTIR) and principal component analysis (PCA) was used to investigate the molecular structure and functional groups present in polyaniline-polyvinyl alcohol-chitosan hydrogels (PAni-PVA-Cs), and to evaluate the contribution of their major chemical components. Identification of composition in an FTIR spectrum is complicated especially when dealing with multicomponent samples where the IR bands can overlap and the spectra of each component are nearly identical. This study focuses on the chemical analysis of the chitosan multi-component system. Specifically, this study aimed to present a novel report on how these components contribute to the chemical features of the blend using PCA. Through the use of the second derivative of the generated SR-FTIR spectra of PVACs hydrogels and iterative curve fitting, the amide II band located at 1658 cm⁻¹ unfolded two peaks located at 1550 and 1569 cm⁻¹ which are associated with intramolecular hydrogen-bonded, intermolecular hydrogen-bonded chitosan. The characteristic peaks of PVA and chitosan were distinguished and located properly by also applying the second derivative and iterative curve fitting in the 800-1125 cm⁻¹ region. The analysis of the PCA of the second derivative transformed SRFTIR spectra of the hydrogels revealed the major contributor to the data variation in the synthesized samples. The generated scatter plots can be inferred that the incorporation of PAni produced a clustering of the samples when the region 800-1800 cm⁻¹ was considered. It also revealed a clustering between the untreated hydrogels and the gamma-irradiated ones on which the loadings imply that the application of gamma radiation affects primarily the pyranose ring skeletal vibrations located at 977 cm⁻¹. The findings support a specific effect of PAni and gamma irradiation on the hydrogels.