

Discrimination of reactive dyes on cotton fabric by raman spectroscopy and chemometrics

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Abstract: FT-Raman spectra were obtained from undyed poplin cotton fabric and from the same fabric differently dyed with a bi-functional reactive dye, Cibacron C (molecular structure unknown); the four series of the dyed samples each contained the dye in a different form-unfixed, ammonia-treated/unfixed, fixed, and ammoniatreated/fixed. The spectra were dominated by the dye, but the different states of the dye were not obviously differentiated. Application of principal component analysis showed that the spectral groups of the four different dye states can be discriminated from each other and from that of the undyed cotton. Further, for each series of the dyed fabrics, which contain samples with different amounts of dye, the individual dye concentration subgroups are distinguished. Exploratory quantitative studies suggested that FT-Raman spectroscopy may be a suitable quantitative method for the prediction of % concentration of the unfixed dye on cotton fabrics. A comparison of the FT-Raman results with those from a parallel FT-IR study reported elsewhere indicated that similar qualitative conclusions may be reached with both techniques. However, the FT-Raman approach does provide additional information from the dominating dye spectrum. A comparison of prediction of % concentration of the unfixed dye on the fabric indicated that better partial least-squares (PLS) calibration models may be obtained from the FT-Raman data, but the validation results from a small set of samples suggested only a marginal advantage with the use of the Raman approach.

Author Keywords: Chemometrics; Cotton-cellulose; FT-Raman spectroscopy; Reactive dyes

Index Keywords: Ammonia; Calibration; Cellulose; Cotton fabrics; Dyes; Mathematical models; Statistical methods; Chemometrics; Fourier transform Raman spectroscopy; Partial least squares (PLS) calibration models; Principal component analysis (PLA); Reactive dyes; Raman spectroscopy

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