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Hyperplane Intercept Vector Calibration Method in Grey Analytical Systems

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A novel vector calibration method, hyperplane intercept, is proposed for grey analytical systems to resolve the concentrations of the chemical components from the multicomponent data gained from attenuated total reflectance-Fourier transform infrared (ATR-FTIR) spectroscopy. This method is capable of quantifying a particular component known to be present in the mixture without having to know the identity of the rest of the components. Through the target factor analysis (TFA), a section of the IR spectrum of the interested component is chosen to calculate the concentration by the proposed hyperplane intercept method. Results calculated from on-line ATR-FTIR spectroscopy data of cyclohexanone ammoximation process are used to illustrate the simplicity and efficiency of this proposed method.

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