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摘要：传统的光谱多元定性方法大都基于主成分分析（PCA），即首先将光谱进行PCA降维并选取特征变量后，再进行聚类或判别分析。近年来，用于光谱多元定量校正的偏最小二乘法（PLS）也被越来越多地用于定性分析中，并得到更优的结果。本文以实例介绍PLS方法在光谱模式识别以及建立定量模型适用性判据等方面的应用，其有望成为一种常用的光谱定性方法。

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The study of use of partial least squares in spectroscopy
qualitative analysis

Abstract: In this paper, the applications of partial least squares method in spectroscopy multivariate qualitative analysis, such as discriminant analysis and outliers detection of quantitative calibration models, were introduced based on several examples. Compared with the traditional principal component analysis method, partial least squares discriminant analysis method usually gives better results.

Key words:

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