激光应用

气溶胶单粒子光谱的PLS聚类分析

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摘要：

PLS聚类法是一种全新的气溶胶单粒子光谱数据处理方法，是利用具有"自组织机制"的PLS(Partial Least Square)回归算法去完成数据的聚类。文中首先阐述了PLS聚类对模拟数据集的运用以展示这种方法的一般特征及有效性，然后应用到气溶胶激光飞行时间质谱数据以展示PLS聚类的正确性及成功运用，最后我们将PLS聚类应用到氯化钙、氯化镁、氯化钠及氯化钾四种气溶胶单粒子激光击穿光谱混合数据集，通过分析聚类获得的树形图和图中节点的统计特性，我们剖析了正确聚类及发生错误划分的原因，表明了PLS聚类方法在气溶胶单粒子谱分析方面的应用潜力。

关键词：　光谱学　偏最小二乘回归　聚类分析　气溶胶单粒子

PLS cluster analysis of Individual particle spectrum

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Abstract:

PLS(Partial Least Squares) cluster analysis, based on PLS regression procedure with a self-organizing mechanism, is a novel data analysis method of spectrum and is. PLS Cluster was first used to classify simulated dataset, and present the general properties and validity. Then it was used to aerosol laser time-of-flight mass spectra data, showing correctness and successful application in practice. Finally, this mothod was applied to mixed spectra dataset of aerosol particles of CaCl2, MgCl2, NaCl and KCl. By examing the statistical properties of obtained dendrogram plots and nodes, we got the reason of clustering and misclassifying. It demonstrates the potency of application of PLS_Cluster in individual aerosol particle spectra.

Keywords: spectroscopy　PLS-regression　cluster analysis　individual aerosol particle

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