化学学报 2000 58 (4): 438-442 ISSN: 1001-604X CN: 31-1547/O6

化学演讲过程数据的自动分辨：复杂石油样品的GC－MS分析

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 基于几种新化学计量学方法，提出了可自动解析化学演进数据的新途径。在该法中，首先选择关键向量。通过子空间比较法确定数据的化学秩。以关键向量为起点，通过初等变换不断迭代而实现对数据的解析。并利用数据非负性等检验解析结果的可靠程度。结合GC－MS数据的特点，选择的关键变量可为关键质谱或关键浓度曲线。该方法能极大地减少人为干预，大大降低数据分析时间，对文中的石油样本共解析出557个成分。

关键词 色谱质谱法 石油 自动分析 关键变量 化学计量学

分类号 064

Automatic resolution of data from evolutionary process: GC-MS analysis of petroleum sample

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Abstract A new procedure, bsed on several recent chemometric method, is proposed for automatic analysis of data from evolutionary process. It runs in the following steps: first, select key spectra or variables; second, determine the chemical rank of data by subspace coparison; third, iterative into pure spectra and concentration profiles by elementary transform. Criteria, e.g. non-negativity, are used to check the reliability of results. As far as data from GC-MS is concerned, key variables can also he used for analysis besides key spectra. The proposed procedure greatly reduces user intervention and therefore saves analysis time. It promises a powerful tool for the resolution of complex system. There are 557 components resolved from petroleum sample in this paper.

Key words CHROMATOGRAPHY-MASS SPECTROGRAPHY PETROLEUM AUTOMATIC ANALYSIS STOICHIOMETRY

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