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基于近红外波长组合快速检测油页岩含油率

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Rapid detection of oil yield of oil shale by combination of wavelengths in near infrared spectroscopy

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摘要　　　　图/表　　　参考文献(0)　　相关文章 (15)

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摘要

为实现油页岩含油率的快速单点测量,研究了基于近红外波长组合的油页岩含油率快速检测方法。以高岭土与机油混合的模拟样品为研究对象,利用便携式近红外光谱分析技术,研究了近红外波长组合选择方法。该方法采用自制的便携式光谱仪获得全光谱反射率数据,结合微分和多元散射校正数据处理及相关系数法进行波长初步筛选,将组合生成算法与留一交互校验多元线性回归(MLR)建模相结合,确定最佳波长组合,并用MLR建模对单点测量获得的最佳波长组合光谱数据进行了实验验证。结果表明:最佳波长组合为1 644,1 720,2 210,2 260 nm,30个建模样品的校正集和预测集的决定系数为0.995 4和0.997 7,11个验证样品的验证集的决定系数为0.990 1。该方法为研制基于单点测量的油页岩含油率快速检测光谱仪提供了基础。

关键词 ： 近红外光谱, 油页岩, 含油率, 波长组合选择, 留一交互校验, 多元线性回归

Abstract ：

To detect rapidly the oil yield of an oil shale on a single point measurement, a detection method was proposed based on combination of wavelengths by a portable near infrared spectroscopy. By taking the kaolin mixed with oil simulating samples as the research object, how to select the combination of wavelengths by near infrared spectroscopy was performed. With proposed method, the full spectral reflectivity data were firstly acquired by the developed portable spectrometer. Then the preliminary selection for the combination of wavelengths was implemented by differential multiplicative scatter correction method and correlation coefficient method, and the optimum combination of wavelengths was determined by combination generation method and leave one cross validation Multiple Linear Regression (MLR). Finally, the data for the optimum combination of wavelengths were verified by MLR modeling. The results show that the optimum combination of wavelengths is 1 644,1 720,2 210 and 2 260 nm, and the determination coefficients for calibration set (R_c^2), prediction set (R_p^2) of 30 modeling samples and validation (R_p^2) of 11 validation samples are 0.995 4,0.997 7 and 0.990 1, respectively. The method provides a basis for design of a rapid detecting spectrometer in oil yields of oil shapes.

Key words ： near-infrared spectroscopy　oil shale　oil yield　combination of wavelengths　leave one cross validation　multiple linear regression

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