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Microscale Organic Maturity determination of Graptolites using Raman Spectroscopy

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Abstract

Organic maturity is a key property for assessment of hydrocarbon potential and generation of black shales. Early Paleozoic strata are usually void of terrestrial organic matter such as vitrinite, thus evading conventional, reflectance based maturity analysis. To overcome this, graptolites in samples from the basal hot shales of the Silurian Qusaiba Formation, with known, reflectance based vitrinite equivalent maturities from 0.54 to 1.98 VRE%, were analyzed with Raman spectroscopy to establish a spectroscopic maturity scale. All samples provided spectra showing the Disorder (D) peak and the Graphite (G) peak typical for organic carbons. Systematic variation of these peaks with sample maturity is used to quantify the relationship of reflectance with the graptolites molecular condition. Several spectral properties were tested for use as maturity indicators. The most reliable maturity tracers are the variation of position of the G peak between 1570 and 1610cm^{-1} and the widening band distance ($\Delta_{(G-D)}$) between the G peak and D peak position at 1320 to 1370cm^{-1}. Comparison of the mean and modal maxima of peak positions showed that the mean of G peak position and $\Delta_{(G-D)}$ provide the best fit of Raman and optical reflectance determinations with R^2 of 0.884 and 0.935, respectively. Algorithms for the calculation of vitrinite equivalent reflectance from the Raman spectral properties were developed based on best fit exponential regressions, with a linear cross correlation of the measured and calculated values at R^2=0.9178 for the mean of $\Delta_{(G-D)}$. Raman based maturity measurements on graptolites provide a welcome alternative method for on particles as small as 3μm diameter.

Keywords: Organic Maturity, Graptolites, Raman Spectroscopy

1. Introduction

Shale-sorbed hydrocarbons have become a significant, “unconventional” global energy resource (e.g., Montgomery et al., 2005; Jarvie et al., 2007). There are many key factors to consider in assessment of shale