Goldschmidt 2022 Abstract
https://doi.org/10.46427/gold2022.9898

Raman spectroscopy of vitrinite-like macerals in the Lower Paleozoic shales

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Vitrinite-like maceral (VLM), an autochthonous type of organic matter with optical features similar to vitrinite, is ubiquitous in many Lower Paleozoic shales. The VLM reflectance ($VLMR_o$) is generally regarded as a proxy of thermal maturity, but its chemical structure and evolution has been little examined. Raman spectroscopy enables direct in-situ analysis of VLM, which can reveal its vibrational microstructural changes.

In this study, the VLM Raman spectroscopy has been applied to natural and artificially-heated immature to over-mature, VLM-rich Lower Paleozoic shales in order to determine its chemical structure and evolution characteristics. The variations of VLM Raman spectra of naturally and artificially-matured shales have been found generally similar. With increasing thermal maturity, the D band position (W_D) shifts significantly towards lower frequency, and the G band position (W_G) shifts slightly towards higher frequency. The width ratio (FWHM-D/FWHM-G), Raman band separation (RBS), and area ratio (A_D/A_G) exhibit positive linear relationships with VLMRo. As the thermal maturity of VLM increases, the oxygen-containing functional groups are being gradually removed, while its aromatic carbon content increases. As the degree of condensation of aromatic rings further proceeds, the lattice defects and aliphatic carbon content diminishes. These changes, notably the increasing aromatization, graphitization, and the growing ordering of VLM, which develop in response to increasing thermal exposure, are remarkably similar to those of classical vitrinite.

The similarities in variations of chemical structure and organic petrological characteristics between VLM and vitrinite confirm that the $VLMR_o$ can be reliably applied to assess the thermal maturity of the Lower Paleozoic shales.

Acknowledgments

This work was supported by National Natural Science Foundation of China (No. 42122016).