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RESEARCH ARTICLE

Thermal Maturity and Structural Characterization of Indian Coals: Insights from Petrographic, Pyrolytic and Spectroscopic Methods

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ABSTRACT

Characterisation of Indian coal samples, collected from various coal-bearing sequences, was performed using spectroscopic techniques (Fourier Transform Infrared and Raman) to understand the structural changes associated with the thermal maturity. The vitrinite reflectance (VR_o%) in the studied samples ranges from 0.28 % to 0.92 % and the T_{max} ranges between 402 ºC and 473 ºC. A strong correlation (R^2=0.95) between VR_o% and T_{max} indicates the reliability of these proxies. The elemental data shows carbon (av. 50.51 wt %), hydrogen (av. 2.78 wt %), nitrogen (av. 0.78 wt %) and sulfur (av. 1.34 wt %) contents. Rock-Eval and Fourier Transform Infrared Spectroscopic (FTIR) parameters collectively suggest the kerogen as Type III. The samples exhibit a range of hydroxyl, aliphatic, aromatic and oxygenated functional groups. FTIR semi-quantitative ratios were applied to examine the compositional variations across the rank, revealing an increase in aromaticity and aromatic ring condensation, as evident from the I_1, C_{ar}/ (C_{ar} + C=O, CH_{ar}/C=C, and H_{ar}/C_{ar} ratios. Additionally, an increase in the aromatic hydrogen content is apparent from the fH and H_{al}/H ratios. The de-functionalisation of oxygenated functional groups is manifested in decrease in the C-factor. Below a VR_o of 0.5%, the samples exhibit consistent behaviour; however, beyond this point, the behaviour becomes abrupt, probably due to the physico-chemical factors controlling the transformations beyond the first coalification jump and/or the diverse origin of the samples. The Raman spectra showed variation of the D-band with respect to VR_o, and the D1A/GA ratio also supports this trend. The hydrogen index (HI) vs. oxygen index (OI) plot showed distinct clustering of the samples according to maturity, suggesting these variations are well-defined across all samples, irrespective of their location and source characteristics.

Keywords: Coal, Vitrinite reflectance, FTIR, Raman spectroscopy, Thermal maturity, Coal structure.

INTRODUCTION

Coal/lignite is an organic-rich sedimentary rock formed by the accumulation of an enormous quantity of vegetal matter, and its subsequent biochemical and physicochemical transformations after deposition (Stach, 1982; Pandey et al., 2024; Zdravkov et al., 2024; Sahu et al., 2025). The physical structure of coal consists mainly of organic material (85-95%) (wt/wt%), inorganic materials (5-15%), and an appreciable quantity of spaces created by the extensive network of pores (Levine, 1982; Ren et al., 2021; Hazra et al., 2025). The chemical structure of coal, however, is highly complex. Since the 1960s, coal chemists have strived to elucidate the essential/fundamental traits of coal organic matter (Marzec, 2002). Generally, the coal structure is composed of clusters of fused and hydrogenated aromatic rings combined by heteroaliphatic or aliphatic chains, creating a three-dimensional network of macromolecular structural units (Ndaji et al., 1997; Izumi et al., 2002; Mathews and Chaffee, 2012). This intrinsic chemical complexity of coal structure arises from multiple sources such as the nature of the original organic matter (OM), preservation and/or selective biodegradation of organic fractions, combined with the physico-chemical processes causing maturation (Lis et al., 2005; Kumar et al., 2024a). The complex macromolecular structure of coal with cross-linked aromatic layers controls key thermochemical conversion properties such as gasification, liquefaction, etc. (Potgieter-Vermaak et al., 2011; Cheng et al., 2022). Further, a deeper understanding of these intrinsic coal properties is crucial for optimising coal conversion and utilisation aspects (Zhang et al., 2015; Liu et al., 2016; Gopinathan et al., 2024; Kumar et al., 2024a, b).

Conventionally, spectroscopic techniques are widely used for the structural characterisation of organic matter. FTIR spectroscopy, in particular, is effective for identifying functional groups based on the