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Evaluating aromaticity changes with thermal stress at the single particle level for a suite of organic matter types from the Boquillas Shale (Texas, United States) via correlative Raman and reflection analyses

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Geochemical, petrographic, and spectroscopic indices that vary with compositional changes in petroliferous organic matter (OM) during thermal maturation are key petroleum system parameters used to understand petroleum generation. In unconventional shale source-rock reservoirs, where multiple, highly dispersed OM types may be present in intimate contact with surrounding mineral phases, OM molecular composition (e.g., aromaticity) is especially useful for informing structure-reactivity relationships representative of different OM types. Here, we employ microscale, in situ, and correlative Raman and reflectance approaches to evaluate aromaticity evolution for a suite of OM types (i.e., liptinite, micrinite, solid bitumen, vitrinite, and inertinite) at the single particle level across an artificial thermal gradient. Our samples include a marginally mature (vitrinite reflectance ~0.5%) Late Cretaceous Boquillas Shale from south Texas, United States, and two hydrous pyrolysis (HP) residues following reaction of the raw Boquillas Shale sample at 300°C and 330°C for 72 hours. Our data indicate that: (i) liptinite, micrinite, solid bitumen, vitrinite, and inertinite particles exhibit different aromatic signatures in the raw shale sample and (ii) these OM types, with the exception of inertinite, effectively experience similar changes in aromatic structure with thermal advance. Data also reinforce the concept that reservoir temperature may be a secondary factor in controlling the molecular composition of inertinite. These findings inform a broader understanding of how different petroliferous OM types evolve throughout thermal reactions and further demonstrate that correlative Raman spectroscopy and reflection analyses, combined with careful organic petrography, can provide complimentary estimates of OM molecular composition and thermal maturity.