Occurrence, composition, and stability of hydrocarbons in deep crustal rocks

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Although most of the organic carbon contained in metasedimentary rocks consists of very mature kerogens (H/C ~ 0.1), significant amounts of extractable hydrocarbons (bitumen) may still be present (e.g. Baker & Claypool, 1970). Demonstrating the syngenicity of this bitumen is of fundamental importance to establish the thermal stability limits of hydrocarbons in ultradeep sedimentary basins (Price, 1993; Schoell & Carlson, 1999), as well as to relate biomarkers extracted from Precambrian rocks to specific metabolisms on the primitive Earth (Peters & George, 2018).

Here we report thermodynamic calculations exploring the relative stabilities of hopanes, steranes, and diamondoid and polycyclic aromatic hydrocarbons in bitumen as a function of temperature, pressure, redox conditions, as well as the compositions of metamorphic kerogens and fluids.

The correct reproduction of isomerizations ratios among methylated naphthalenes (MNR, DNR) and phenanthrenes (MPR), and among methyladamantanes (MAI) in bitumen under metamorphic conditions (deduced from mineralogical assemblages or vitrinite reflectance and fluid inclusion data) suggests that at least the aromatic fractions of the bitumens are indeed syngenetic (Brocks *et al*., 2003; Schwab *et al*., 2005). In contrast, the results of the calculations indicate that steranes and hopanes should not be found in detectable concentrations in rocks which have experienced temperatures in excess of ~ 200°C.

References

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