Thermodynamic studies of water-rock-hydrocarbon-gas interactions in petroleum systems

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The thermodynamic database for hydrocarbons of interest to petroleum geochemistry, which was constituted twenty years ago (1,2), has been extensively revised and expanded, and is currently applied to develop quantitative models exploring the evolution of petroleum systems (i.e. reservoir and source rocks) as a function of the temperature, pressure, and redox conditions typical of sedimentary basins. The revision of the original thermodynamic database was deemed necessary after the appearance of new calorimetric studies and, in the case of polycyclic aromatic hydrocarbons (PAH), the recognition that group additivity estimates of their thermodynamic properties (2) were not precise enough for geochemical calculations (e.g. isomerization ratios as a function of maturity or absolute concentrations of PAH in crude oils). A new approach has therefore been developed to refine the group additivity predictions, which relies both on calorimetric data and geochemical observations. In a sense, this approach is similar to that used in metamorphic petrology to derive thermodynamic properties of minerals from reversal experiments.

A number of geochemical applications of the revised thermodynamic database will be presented, including:

- the stability of hydrocarbons at high temperatures,
- thermochemical sulfate reduction (3),
- the evolution of kerogen towards graphite during metamorphism (4).

The consequences for the geochemical cycle of organic carbon in deep sedimentary basins and the presence of organic compounds in metamorphic rocks will be discussed.

References

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