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Calculation of thermodynamic functions for hydrocarbons and their mixtures JEFFERY PERKINS, JASON HO, University of the Fraser Valley, NOHAM WEINBERG, University of the Fraser Valley, Simon Fraser University — Knowledge of thermodynamic parameters of oil components in their pure forms and in mixtures is vital to understanding the properties of petroleum. The fact that hydrocarbons, thermodynamically unstable at ambient conditions, are formed spontaneously at geochemical conditions from a variety of precursors, ranging from kerogen to carbon, suggests that the thermodynamic stability of hydrocarbons increases dramatically with increasing pressure and temperature. Better grasp of their thermodynamic properties at extreme conditions is therefore crucially important both for our understanding of the processes of oil formation and for our ability to design and engineer new methods of synthetic oil production. Unfortunately, with a very few exceptions of the simplest compounds, such as e.g. methane, ethane, or ethene, these properties are tabulated for rather narrow ranges of pressures and temperatures, and in most cases are listed only for standard conditions at 25°C. We propose a new computational methodology, based on classical molecular dynamics simulations, for obtaining accurate thermodynamic functions, such as Gibbs energies, entropies, and enthalpies, of oil components and their mixtures at elevated and extreme temperatures and pressures.

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