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Theoretical Tools for the Analysis and Prediction of Multi-component Systems at High Pressures and Densities J. F. KENNEY, A.P.S. — J. F. Kenney, Gas Resources Corporation, Houston, Texas, U.S.A. To describe or predict theoretically the evolution of a multi-component system at high pressures, one must have a reliable expression for the system's partition function, or its Helmholtz free energy, or its equation of state. Such formalism must possess the following properties: The formalism must be based upon fundamental, first-principles, quantum statistical mechanics argument, and the highest level of rigor available; it cannot be *ad hoc*, or use fitted expressions; the equation of state developed by the formalism must be generate accurately, not only the system's basic pressure-density relationship, but also its multi-phase transition and coexistence lines, and its complex-behavior curves; and it must include also an adequate optimization procedure capable to determine the equilibrium state of the system. Here is described a general formalism that has been used to describe high pressure systems and has resolved the previously-outstanding problems of optical activity in abiological compounds, the anomalous distribution of isomers in petroleum, and the spontaneous generation of the hydrocarbon system.

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