Thermodynamic Properties of Solid and Liquid Methane. Theory and Computer Simulation

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Wide application of methane and its derivatives in low-temperature technology as well as recently discovered presence of condensed methane on surfaces of several celestial bodies make it essential to understand its thermophysical properties in wide ranges of temperature and pressure. Location of the methane melting line was recently theoretically predicted using two equations of state: for the fcc-solid and liquid phases [1]. Equations of state for both phases were constructed in the framework of perturbation theory using reference system build of spherical molecules, for both crystal and liquid phases, and the octupole - octupole interaction of methane molecules as a perturbation. The reference system for the solid phase was described using a canonical equation of state, based on a generalization of Mayer's group expansion on solids [3]. In this paper, we present results of new Monte Carlo computer simulations of the same system and compare their results with calculations based on a perturbation theory equation of state and available for the high-temperature phase of methane experimental data. The contributions of the octupole - octupole and short-range atom-atom interactions to different thermodynamic properties of solid and liquid phases of methane are estimated and discussed.

References

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