Accurate *Ppt* Data for Argon from Monte Carlo Simulations Using *Ab Initio* Two-Body and Nonadditive Three-Body Potentials

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Monte Carlo simulations allow for the calculation of accurate thermodynamic properties of a substance provided that the true intermolecular potential energies are known. We have performed Monte Carlo simulations in the isothermal-isobaric ensemble for argon covering a wide range of density along subcritical and supercritical isotherms. We utilized the accurate *ab initio* potentials of Jäger et al. for the pair interaction energies [1] and the nonadditive three-body contributions [2]. Quantum effects were accounted for by using the quadratic Feynman-Hibbs effective pair potential [3]. Comparison with the best experimental data [4] gives proof to the high accuracy of our results for the gas, liquid, and supercritical phases. We also demonstrate the effects on the results when exchanging the three-body potential for a simple Axilrod-Teller-Muto potential, and what happens when the three-body contributions or the quantum corrections are neglected. We conclude that our approach is able to add accurate values for thermodynamic properties to the available experimental data, especially at extreme temperatures and pressures, and we are confident that it provides the foundation for constructing reliable fundamental equations of state from pure theory for substances where experimental data are difficult to obtain.

References

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