

Abstract Submitted  
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**Estimates of vapor pressure below the triple point for the LJ system** BARBARA N. HALE, Missouri University of Science & Technology — Vapor pressures are estimated for a full Lennard-Jones (LJ) potential system at three temperatures below the triple point. A Bennett Monte Carlo calculation of Helmholtz free energy differences for small LJ  $n$ -atom clusters is used to predict  $\ln(\rho_{liq}/\rho_1)$ , the intercept at  $n = \infty$ , where  $\rho_{liq}$  and  $\rho_1$  are bulk liquid and monomer vapor number densities. The approximation that the vapor consists of monomers only provides an estimate of  $\ln(P)/P_c$ . The results are presented in a corresponding states plot comparison with experimental data for argon at higher temperatures, the extrapolated vapor pressure formula used by Iland *et al* [K. Iland, J. Wölk and R. Strey, *J. Chem. Phys.* **127**, 54506 (2007)], and Monte Carlo results of Chen *et al.* [B. Chen, J. I. Siepmann, K. J. Oh, M. L. Klein, *J. Chem. Phys.* **115**, 10903 (2001)] Such a plot provides a check on vapor pressure expressions extrapolated to low temperatures where no experimental data are available.

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