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# Lennard-Jones and Devonshire Equation of State at Low Temperatures

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In recent years it has become increasingly apparent that the Lennard-Jones and Devonshire (LJD) model of molecular assemblies[1] is more appropriate to the solid state than to the liquid.[2] For this reason we have considered it worthwhile to extend the existing tabulations of the LJD equation of state[3,4] to the region of low reduced temperatures in which the solid is the stable form. We have followed the method of Wentorf *et al.*,[3] and in this note we have employed their system of symbols without redefinition.

The main part of the computations consisted in evaluating the integrals $G$, $g_L$, $g_M$ [Eqs.(5)–(7) of reference 3], whose integrands at first increase steeply with increasing values of the variable $y$, reach a maximum, and then decrease more slowly. The integrations were carried out numerically using Simpson's rule and taking 80–90 values of the integrand. They were usually divided into three parts, the main one integrating through the peak of the integrand from 1/5 its height on one side to about the same height on the other, taking 60 intervals. Two subsidiary parts of 10–20 intervals evaluated (a) the "tail" of the curve, and (b) the initial steep portion down to a value of $y$ for which the exponential factor in the integrand was very close to unity and the integration could be performed analytically. The results[5] are presented in Table I in the form of a tabulation of the "compressibility factor" $pv/NkT$ at particular values of the reduced volume $v/v_0$ and temperature $kT/\epsilon_m$. It should be noted that

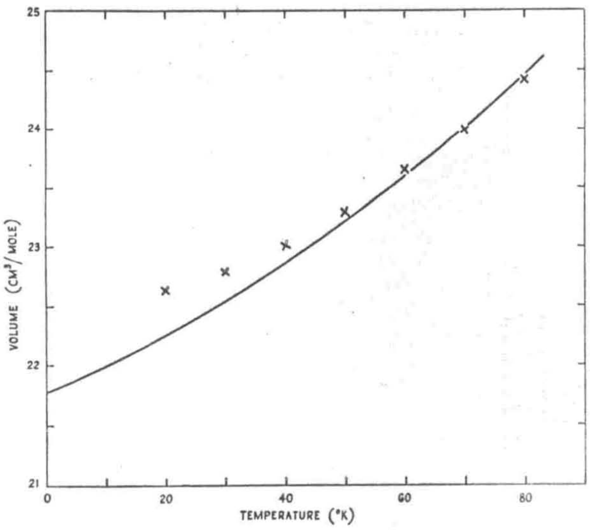


FIG. 1. The volume of solid argon (at its normal vapor pressure) as a function of the temperature. The crosses are experimental values,[7] and the curve is given by the LJD theory.

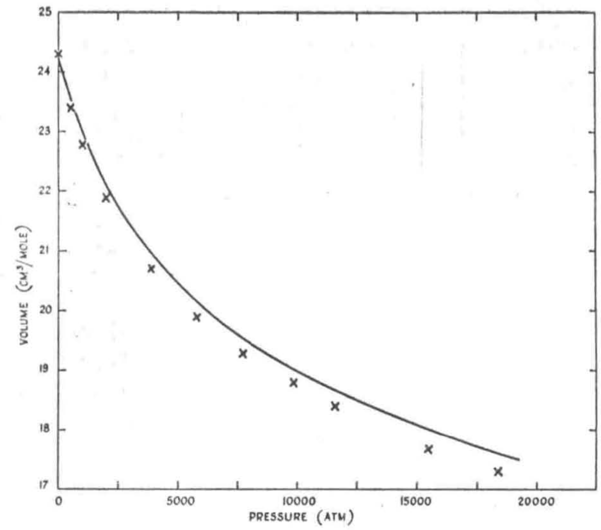


FIG. 2. The volume of solid argon at 77°K ($kT/\epsilon_m=0.643$) as a function of the pressure. The crosses are experimental values,[8] and the curve is given by the LJD theory.