

TABLE I. Values of the factor $\rho v/NkT$.

| $v/v_0 \diagdown kT/\epsilon_m$ | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
|---------------------------------|--------|--------|--------|--------|---------|---------|---------|--------|--------|--------|
| 0.30 | 26749 | 13378 | 8921 | 6693 | 5356 | 4464 | 3827 | 3350 | 2978 | 2681 |
| 0.35 | 13816 | 6911 | 4610 | 3459 | 2769 | 2309 | 1980 | 1733 | 1541 | 1388 |
| 0.40 | 7678 | 3843 | 2564 | 1925 | 1541.4 | 1285.7 | 1103.1 | 966.1 | 859.6 | 774.3 |
| 0.45 | 4497 | 2252 | 1503.8 | 1129.6 | 905.2 | 755.5 | 648.6 | 568.5 | 506.1 | 456.2 |
| 0.5657 | 1473.5 | 740.4 | 496.2 | 373.9 | 300.7 | 251.8 | 216.9 | | | |
| 0.6364 | 773.1 | 390.4 | 262.7 | 198.9 | 160.6 | 135.2 | 116.9 | | | |
| 0.7071 | 399.8 | 203.9 | 138.5 | 105.9 | 86.09 | 72.96 | 63.67 | | | |
| 0.8485 | 75.02 | 41.63 | 30.47 | 24.80 | 21.45 | 19.19 | 17.52 | | | |
| 0.9899 | -32.95 | -12.01 | -5.159 | -1.801 | 0.1466 | 1.449 | 2.372 | | | |
| 1.0607 | -55.23 | -23.03 | -12.44 | -7.246 | -4.174 | -2.200 | -0.8034 | | | |
| 1.1314 | -66.97 | -28.77 | -16.17 | -10.03 | -6.450 | -4.105 | -2.467 | | | |
| 1.5556 | -57.61 | -25.01 | -14.47 | -9.343 | -6.345 | -4.393 | -3.029 | | | |
| 1.9799 | -34.89 | -15.58 | -9.104 | -5.870 | -3.940 | -2.664 | -1.761 | | | |
| 2.1213 | -30.70 | -13.72 | -8.012 | -5.149 | -3.433 | -2.295 | -1.487 | | | |
| 2.4749 | -24.09 | -10.71 | -6.211 | -3.945 | -2.582 | -1.671 | -1.022 | | | |
| 2.8284 | -20.33 | -8.965 | -5.148 | -3.226 | -2.066 | -1.291 | -0.7379 | | | |
| 3.5355 | -16.14 | -7.004 | -3.938 | -2.395 | -1.465 | -0.8433 | -0.3990 | | | |
| 4.2426 | -13.69 | -5.851 | -3.218 | -1.893 | -1.096 | -0.5637 | -0.1844 | | | |
| 5.0 | -11.89 | -4.994 | -2.678 | -1.524 | -0.8435 | -0.4037 | -0.1019 | 0.1145 | 0.2747 | 0.3966 |

our data overlap those of Wentorf *et al.*³ at $kT/\epsilon_m = 0.7$, and that the agreement is satisfactory.

We have used these data to calculate theoretical volume-temperature and volume-pressure relationships for solid argon, converting the reduced volumes and temperatures of the LJD theory to absolute units by the factors $v_0 = 23.78 \text{ cm}^3/\text{mole}$, $\epsilon_m/k = 119.8^\circ\text{K}$, derived from the second virial coefficient of gaseous argon.⁶ Our results are compared with experimental data in Figs. 1⁷ and 2.⁸ It will be seen that the LJD theory gives a good description of the actual volumetric behavior of solid argon over a wide range of conditions.⁹ The failure of the theory at the lowest temperatures⁸ (Fig. 1) is probably the result of its being based on a classical and not a quantal model.

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¹ J. E. Lennard-Jones and A. F. Devonshire, Proc. Roy. Soc. (London) **A163**, 53 (1937).

² See, particularly, J. A. Barker *Lattice Theories of the Liquid State* (Pergamon Press, Ltd., London, 1962).

³ R. H. Wentorf, Jr., R. J. Buehler, J. O. Hirschfelder, and C. F. Curtiss, J. Chem. Phys. **18**, 1484 (1950).

⁴ W. Fickett and W. W. Wood, J. Chem. Phys. **20**, 1624 (1952).

⁵ To save space we have not included tables of the integrals G , g_L , g_M , although they are useful for deriving the energy and entropy of imperfection. They are available on request.

⁶ J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954), p. 1110.

⁷ E. R. Dobbs and G. O. Jones, Rept. Progr. Phys. **20**, 516 (1957).

⁸ J. W. Stewart, J. Phys. Chem. Solids **1**, 146 (1956).

⁹ It should be emphasized that the *only* experimental property of argon introduced into the calculations is its second virial coefficient.