

TABLE I. Values of the factor pv/NkT .

$\frac{kT}{\epsilon_m}$ v/v_0	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 temperatures⁶ (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. Buchler, J. O. Hirschfelder, and C. F. Curtiss, *J. Chem. Phys.* **18**, 1484 (1950).

⁴ W. Fickert 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.