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by

G. I. Kerley

A THEORETICAL EQUATION OF STATE FOR DEUTERIUM

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ABSTRACT

The thermodynamic properties of deuterium are calculated for densities ranging from 10^{-3} to 10^{3} gm/cm^{3} and for temperatures ranging from 200 to 10^{6} °K. Phase transitions between the molecular solid, metallic solid, and fluid phases are determined. Effects of dissociation and ionization are included in the fluid equation of state. Tabular results are presented for deuterium only, but approximate equations of state for hydrogen and tritium can be obtained by scaling the deuterium data.

I. INTRODUCTION

In this report, we describe an equation-of-state calculation for deuterium over a wide range of densities and temperatures. This work was undertaken for practical reasons as well as for its inherent theoretical interest.

Because deuterium is a source of fusion power, its equation of state is needed in the analysis of thermonuclear systems, including weapons, fusion reactors, and stars. In addition, equation-of-state information is useful in the study of the planets Jupiter and Saturn, which contain large concentrations of very dense hydrogen.[1] We choose to do our calculations for the deuterium isotope because of interest in the fusion problem. However, the theory is just as applicable to hydrogen and tritium. As a rough approximation, equations of state for these isotopes can be obtained by scaling our deuterium data.

Deuterium is also interesting from a theoretical point of view. Although it might seem to be a simple substance, deuterium poses nearly all of the difficulties that arise in equation-of-state theory. The list of problems includes fluid and solid theory, molecular and metallic binding, phase transitions, molecular vibration and rotation, and chemical reactions (dissociation and ionization). Previous calculations, in which some of these problems have been ignored, are only applicable within a limited range of densities and temperatures. Treatment of the fluid phase has been particularly weak. We hope that the theoretical models developed in this study will also be useful in calculations for other materials.

In this report, primary emphasis is given to the properties of the fluid phase. Because of dissociation and ionization, the fluid is a rather complicated mixture of molecules, atoms, protons, and electrons. To simplify the problem, we derive separate equations of state for the pure molecular gas and the pure atomic gas. These calculations, which are discussed in Section V, employ the CRIS fluid model, which was described in a previous report.[2] These results are combined, and the fraction of dissociation is determined by an equilibrium calculation as described in Section IV. We also assume that vibration-rotation effects (Section VI) and thermal electronic excitations (Section VII) can be separated from translational contributions to the equation of state. We do not consider the gas-liquid coexistence region, because the critical temperature is only 33°K, well below the range of our table.

In addition to the fluid phase, we assume that there are two solid phases of deuterium -- a molecular form, which we calculate to be stable at pressures below about 2 mbar, and a metallic form, stable at high pressures. An equation of state for the molecular solid is derived in Section II, using the Lennard-Jones and Devonshire theory.[3] The metallic modification is treated as a Debye solid, as described in Section III.[4] The phase diagram, including a fluid region and two solid regions, is discussed in Section VIII, using standard thermodynamic arguments.

Although numerous approximations are made throughout this report, we try to consider each of the important problems mentioned above so that the equation of state can be specified at any density and temperature. However, certain problems which are important at low temperatures, such as critical phenomena, nuclear spin statistics, hindered rotation in the solid state, and some quantum effects, are neglected. For this reason, our table does not go below a temperature of 178°K.

Some of the results for the pressure, internal energy, and Helmholtz free energy, as functions of density and temperature, are given in Table II. A more extensive table is presently in use at this Laboratory.

In a previous report, the CRIS fluid model was shown to agree very well with Hugoniot measurements and other experimental data for hydrogen and deuterium.[2] Those comparisons are not repeated here. Other tests of our equation of state will be discussed in future reports, as new experimental data become available.

II. THE MOLECULAR SOLID

In this section we calculate the thermodynamic properties of solid molecular deuterium from the cell model of Lennard-Jones and Devonshire (LJD).[3] Although the LJD model was originally proposed as a theory of the liquid state, experience has shown that it actually describes a solid. In a previous report, we demonstrated that the LJD model, together with our CRIS model of fluids, gives very good predictions for the melting and sublimation curves of argon.[2]

We assume that the Helmholtz free energy of the solid can be written

$$A(V,T) + E_c(V) + A_N(V,T) + A_{VR}(V,T), \qquad (1)$$

where $E_c(V)$ is the cohesive energy of the solid at 0°K, A_N is the translational free energy of the nuclei, and A_{VR} is the free energy of vibration and rotation. In both solid and fluid phases, we ignore excited electronic states of the molecule, which should make a negligible contribution to the equation of state. The vibrational-rotational degrees of freedom are assumed to be separable from the translational motion and are discussed in Section VI.

The LJD model is based upon the assumption of additive pair potentials between molecules. At high densities, where some delocalization of the electrons can occur, provision must be made for non-additive effects. Instead of calculating the zero-temperature isotherm from the potential function, we use the following analytic expression.

$$E_c(V) = 246.66\ F\ (F - 2)\ {}^{\circ}K,$$

$$F = \frac{19.197\ \eta^{1/3}}{(1 + .4286/\eta^{4/3})(1 + 4.0201/\eta)(1 + 1.6767/\eta^{1/3})}, \qquad (2)$$

where $\eta = 15.9/V$, and V has units of cm^3/g-mole. Equation (2) was derived in a previous report,[2] by fitting the compressibility measurements of Stewart[5] at low densities and the band theory calculations of Liberman[6] at high densities. It should be noted that Eq. (2) does not include any contribution from the zero-point energy of lattice vibrations, so that our solid model is inadequate at low temperatures. However, our previous calculations on argon indicate that it is safe to ignore quantum effects at room temperature and higher. Equation (2) is also used in the fluid model, Section V.

According to the LJD theory, the translational free energy of the solid is

$$A_N(V,T) = A_o(V,T) + NkT\ [1 - \ln\ (Nv_F/V)], \qquad (3)$$

where A_o is the free energy of an ideal gas and v_F is the free volume. A_o is given by

$$A_o(V,T) = NkT\ [7.0719 - \ln V - \frac{3}{2}\ \ln\ (MT)], \qquad (4)$$

where V is the volume in cm^3/mole, T is the temperature in °K, and M is the molecular weight in g /mole. The free volume is calculated by assuming that a molecule is surrounded by 12 nearest neighbors which are smeared out over a spherical shell of radius $a = 2^{1/6}(V/N)^{1/3}$. The result is[3]

$$v_F = 4\pi \int_0^{r_M} r^2 \exp\left[-\frac{E(r) - E(o)}{kT}\right] dr,$$

$$E(r) = 6 \int_{-1}^{1} \phi\left(\sqrt{r^2 - 2\, ar \cos\theta + a^2}\right) d\cos\theta \ , \qquad (5)$$

where $r_M = (3V/4\pi N)^{1/3}$, and $\phi(R)$ is the potential function for the interaction of two molecules. In this work we treat the molecules as if they were spherically symmetric. For the free volume calculation, the assumption of additive pair potentials is a satisfactory approximation, because we are only interested in the deviation in energy as two molecules are simultaneously displaced from their equilibrium positions in the lattice. Moreover, at the high densities where non-additive effects become important, the translational contributions are small when compared with the zero-temperature isotherm.

Quantum-mechanical calculations of the potential between two hydrogen molecules have been made by several authors.[7-13] Neece et al.[8] used the valence bond calculations of Magnasco and Musso[9] for the repulsive contribution to the potential, and the calculations of Margenau[10] for the attractive contribution. However, their potential overestimates the repulsive forces, and their equation-of-state calculations do not agree with Stewart's measurements[5] at low density. Other authors have treated the pair of molecules as a cluster of four separate atoms.[11-13] According to this "separate atom" model, the potential, $\phi_A(R)$, between two atoms in different molecules is[12]

$$\phi_A(R) = \frac{1}{4}\,[E_s(R) + 3E_t(R)] \ ,$$

where E_s is the energy of the singlet state of the H_2 molecule and E_t is the energy of the triplet state. Unfortunately, this procedure is subject to large errors because of uncertainties in the functions $E_s(R)$ and $E_t(R)$. In this work we use the potential proposed by Trubitsyn,[13] because it fits Stewart's measurements for deuterium and agrees fairly well with our zero-temperature isotherm at higher densities. For ease in the calculations, Trubitsyn's potential can be fit to the following simpler form.

$$\phi(R) = \epsilon\left[e^{B(1 - R/\sigma)} - e^{C(1 - R/\sigma)}\right] \ , \qquad (6)$$

where $\epsilon = 140^\circ K$, $\sigma = 2.987$ Å, $B = 10.217$, and $C = 6.855$. Using Eq. (6), the free volume can be written

$$\frac{Nv_F}{V} = 2\sqrt{2\pi} \int_0^{y_M} y^{1/2}\, e^{-F(y)}\, dy \ ,$$

$$F(y) = C_2\left[C_3 \frac{\sinh\,(C_1 y^{1/2})}{C_1 y^{1/2}} - \frac{\cosh\,(C_1 y^{1/2})}{C_1} - 1\right] - C_5\left[C_6 \frac{\sinh\,(C_4 y^{1/2})}{C_4 y^{1/2}} - \frac{\cosh\,(C_4 y^{1/2})}{C_4} - 1\right], \qquad (7)$$

where $y_M = (3/4\sqrt{2\pi})^{2/3}$ and the constants are given by

$$C_1 = 2^{1/6}\, B\, (V/N\sigma^3)^{1/3} \ ,$$

$$C_2 = \frac{12\epsilon}{T}\, e^{B} - C_2 \ ,$$

$$C_3 = 1 + 1/C_2 \ ,$$

$$C_4 = 2^{1/6}\, C\, (V/N\sigma^3)^{1/3} \ ,$$

$$C_5 = \frac{12\epsilon}{T}\, e^{C} - C_2 \ ,$$

$$C_6 = 1 + 1/C_5 \ .$$

Finally, the energy and pressure of the solid molecular phase are given by

$$E(V,T) = E_c(V) + \frac{3}{2} NkT + NkT^2\left[\frac{\partial \ln(Nv_F/V)}{\partial T}\right]_V + E_{VR}(V,T) \ , \qquad (8)$$

$$P(V,T) = -\frac{dE_c}{dV} + \frac{NkT}{V} + NkT\left[\frac{\partial \ln(Nv_F/V)}{\partial V}\right]_T$$

$$+ P_{VR}(V,T) \quad , \qquad (9)$$

where E_{VR} and P_{VR} are the contributions from vibration and rotation (Section VI).

III. THE METALLIC SOLID

It is generally assumed that, at high pressure, solid hydrogen and deuterium undergo a first-order phase transition from the molecular form to a metallic modification, having one atom per unit cell. Numerous calculations of the cohesive energy of the metallic form have been made.[1, 8, 12-20] Estimates of the transition pressure range from .25 to 20 mbar. In this work we calculate the equation of state for the metallic solid from the Debye theory, using a cohesive energy curve based upon the results of Neece et al.[8]

We assume that the Helmholtz free energy of the metallic solid can be written

$$A(V,T) = E_c(V) + A_N(V,T) + A_e(V,T) \quad , \qquad (10)$$

where $E_c(V)$ is the cohesive energy of the solid at 0°K, A_N is the free energy of lattice vibrations, and A_e is the contribution of excited electronic states and ionization to the free energy. Calculation of the electronic terms is discussed in Section VII.

In previous work at this Laboratory, we have found the following analytic expression to give a satisfactory fit of zero-temperature isotherms for most materials.

$$E_c(V) = E_B\, F\,(F - 2) \ ,$$

$$F = \frac{D\eta^{1/3}}{(1 + B/\eta)(1 + A/\eta^{2/3})(1 + C/\eta^{1/3})} \quad , \qquad (11)$$

where $\eta = V_o/V$ and E_B is the binding energy when $V = V_o$. Bardeen has shown that the cohesive energy approaches the following form at high densities.[21]

$$E_c(V) \longrightarrow \frac{2.21\ a_o^2}{r_s^2} - \frac{3a_o}{r_s} + I \ \text{Rydberg}, \qquad (12)$$

where a_o is the Bohr radius (.5292 Å), $r_s = (3V/4\pi N)^{1/3}$ is the Wigner-Seitz cell radius, and I is the ionization energy of the atom (13.6 eV for hydrogen). Requiring that Eq. (11) approach the limit of Eq. (12) as $V \rightarrow 0$, together with the condition that $F(V_o) = 1$, we obtain the following relations.

$$D = \left[\frac{1.8105 \times 10^5}{E_B\, V_o^{2/3}}\right]^{1/2} \ ,$$

$$C = .94215\ V_o^{1/3} - 1/D \ ,$$

$$A = 1.5\ C^2 + C/D - .43593\ V_o^{2/3} \ ,$$

$$B = \frac{D}{(1 + A)(1 + C)} - 1 \quad , \qquad (13)$$

where E_B has units of $^\circ$K, and V_o has units of cm^3/g-atom. With this simple prescription, all we require to specify the cohesive energy curve are values of E_B and V_o. It is impossible to determine which of the available calculations is best. In this work we use the results of Neece et al., who used a self-consistent treatment including correlation effects.[8] Their computational method was shown to work well for lithium and sodium. If zero-point energy is not included, these authors predict a binding energy of .073 Ry at 1.771 cm^3/g-atom. To calculate the zero-point energy for deuterium, their expression for the Debye temperature for hydrogen must be divided by a factor of $\sqrt{2}$. The resulting equation-of-state parameters are given in Table I, and the cohesive energy curves are shown in Fig. 1. The cohesive energy curve without zero-point energy is used in the fluid model (Section V).

TABLE I

EQUATION OF STATE PARAMETERS FOR METALLIC DEUTERIUM

	Without ZPE	With ZPE
$E_B(^{o}K)$	1.1523×10^4	9.8648×10^3
$V_o(cm^3/g\text{-atom})$	1.771	1.8583
A	0.66162	0.72997
B	0.0747	0.07638
C	0.83465	0.87133
D	3.2762	3.4846

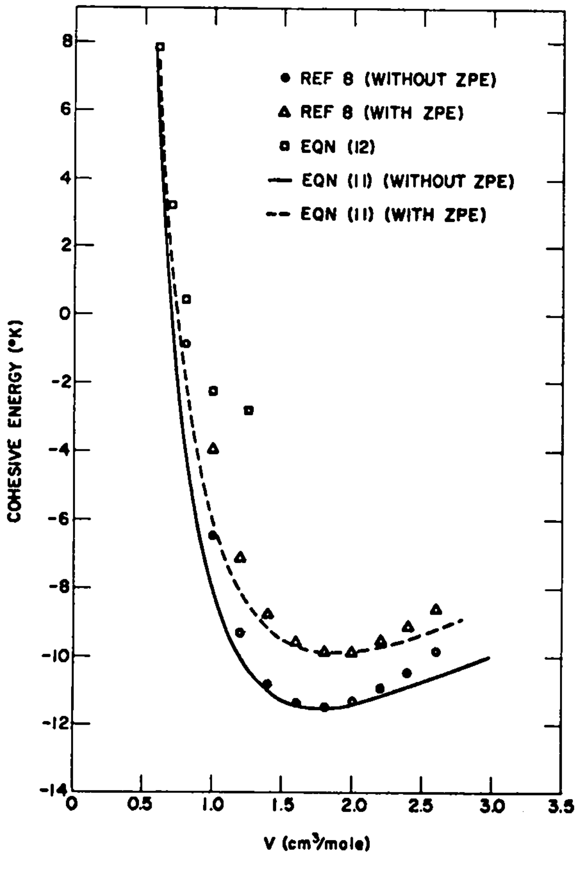

Fig. 1. Cohesive energy curves for solid metallic deuterium.

According to the Debye model, the free energy of lattice vibrations is[4]

$$A_N(V,T) = NkT\left[3\ln\left(1 - e^{-\theta/T}\right) - D(\theta/T)\right] ,$$

$$D(\theta/T) = \frac{3T^3}{\theta^3}\int_0^{\theta/T} \frac{x^3dx}{e^x-1} , \qquad (14)$$

where θ is the Debye temperature. θ is related to the Grüneisen function, $\gamma(V)$, by

$$\theta(V) = \theta_o \exp\left(-\int_{V_o}^{V} \gamma(V)\,\frac{dV}{V}\right). \qquad (15)$$

The Grüneisen function can be estimated from the zero-temperature isotherm by the Dugdale-MacDonald relation[22]

$$\gamma(V) = -\frac{1}{6} - \frac{1}{2}\,\frac{V^2(dP_c/dV) + \frac{5}{3}V(dP_c/dV)}{V(dP_c/dV) + \frac{2}{3}P_c} , \qquad (16)$$

where $P_c = -dE_c/dV$. For θ_o, we use the expression

$$\theta_o = \frac{h}{3\pi k}\left(\frac{6\pi^2}{NV_o^{\,2}}\right)^{1/3}\sqrt{\frac{1}{M}\left(-\frac{dP_c}{dV}\right)_{V_o}} . \qquad (17)$$

Equation (17) follows from the derivation of Slater,[4] if Poisson's ratio is taken to be 1/3, in accordance with most results for solids.

Finally, the energy and pressure of solid metallic deuterium are calculated as follows.

$$E(V,T) = E_c(V) + 3NkT\,D(\theta/T) + E_e(V,T) , \qquad (18)$$

$$P(V,T) = -dE_c/dV + 3\gamma\,\frac{NkT}{V}\,D(\theta/T) + P_e(V,T), \qquad (19)$$

where E_e and P_e are the electronic contributions (Section VII).

IV. THE FLUID PHASE AND DISSOCIATION

In this section we discuss the effects of chemical equilibrium on the thermodynamic properties of the fluid phase. In order to simplify the problem, we consider only dissociation and ionization. Hence the only chemical species assumed to be present are D_2, D, D^+ (deuterons), and e^- (electrons). It is doubtful that other species, such as D_2^+, are ever found in a high enough concentration to affect the equation of state. Since we ignore the molecular ion, D_2^+, a molecule cannot ionize without first dissociating, and ionization can be considered along with the other electronic contributions to the atomic equation of state (see Section VII).

In general, the fluid phase is a complex mixture of molecules and atoms. Since no adequate theory of mixtures exists at the present time, it is necessary to make simplifying assumptions. For an ideal gas, the partition function for the mixture is[23]

$$Q(V,T) = \frac{1}{(1 - f)^{(1 - f)N} f^{2fN}} \; q_M^{(1 - f)N} \, q_A^{2fN} \, e^{-fND_0/kT} , \qquad (20)$$

where N is the number of molecules present before dissociation, f is the fraction of molecules which are dissociated, and D_o is the dissociation energy. q_M and q_A are the partition functions for a molecule and atom, respectively. The Helmholtz free energy of the mixture is

$$A(V,T) = (1 - f) \, A_M(V,T) + f \, A_A(V,T) + fND_o + (1 - f)NkT \ln(1 - f) + 2f \, NkT \ln f, \qquad (21)$$

where A_M and A_A are the free energies for a pure molecular gas and a pure atomic gas, respectively. For ideal gases, A_M and A_A depend only on V and T, and not on the composition of the system. For real gases, A_M and A_A should also depend upon f, because of the interaction between molecules and atoms. However, we will ignore this complication in our calculations, and use values of A_M and A_A, determined for the pure components as described in Section V. Notice, however, that our expressions for the quantities A_M and A_A are those for real gases, not those for ideal gases.

The fraction of dissociation is obtained by minimizing the free energy with respect to f. The result is

$$\frac{ef^2}{1-f} \exp\left(\frac{A_A + D_o - A_M}{NkT}\right) = 1 . \qquad (22)$$

Once Eq. (22) has been solved for f, the energy and pressure are calculated from the formulas

$$E(V,T) = (1 - f) \, E_M(V,T) + f \, E_A(V,T) + f \, D_o ,$$

$$P(V,T) = (1 - f) \, P_M(V,T) + f \, P_A(V,T) , \qquad (23)$$

where E_M and P_M are the energy and pressure of a pure molecular gas, and E_A and P_A are the energy and pressure of a pure atomic gas.

In Fig. 2 we show the fraction of dissociation as a function of density and temperature. At low densities, molecules tend to recombine as the density increases, in accordance with Le Chatelier's principle. At high densities this trend is reversed, because the atomic gas becomes more stable than the molecular gas. In the high-density region, our calculation shows a tendency for molecules to recombine as the temperature increases. This result, which seems unlikely from an intuitive point of view, is probably due to approximations in our treatment of the mixture problem and in the vibrational-rotational degrees of freedom (see Section VI). However the effect is small and can be ignored.

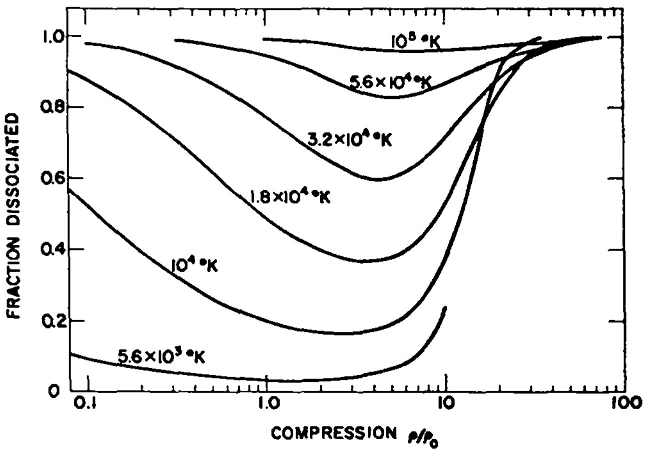

Fig. 2. Fraction of dissociation in fluid equation of state. The compression is ρ/ρ_0, where ρ is the density and ρ_0 = .17 g /cm^3.

V. THE FLUID MODEL

The CRIS model, a theory for calculating the thermodynamic properties of a fluid from the zero-temperature isotherm of the solid and the hard-sphere equation of state, was discussed in a previous report.[2] The theory was used, with great success, to calculate the thermodynamic properties and Hugoniots of fluid argon and hydrogen, and also the melting, sublimation, and gas-liquid coexistence curves of argon. In this work we use a slight modification of this theory to calculate the properties of both the molecular and atomic fluids. For a more detailed discussion of the model, the reader should refer to LA-4760.

According to the theory, the translational contribution to the Helmholtz free energy is given by

$$A(V,T,\eta) = A_0(V,T) + NkT\,\alpha(\eta) + N\,\varphi(V,\eta) \quad ,$$

$$\eta = NR_0^3/\sqrt{2}\,V \quad , \qquad (24)$$

where R_0 is an effective hard-sphere diameter for a fluid atom. A_0 is the free energy of an ideal gas, given by Eq. (4), $NkT\,\alpha(\eta)$ is the excess free energy of a hard-sphere fluid, and $\varphi(V,\eta)$ is the average energy of a fluid atom. The packing fraction, η, is a parameter which characterizes a family of fluid structures; it is determined as a function of V and T by minimizing the Helmholtz free energy.

$$\left[\frac{\partial\, A(V,\,T,\,\eta)}{\partial\eta}\right]_{V,T} = 0 \quad . \qquad (25)$$

Once η has been calculated from Eq. (25), the energy and pressure are determined as follows.

$$E(V,T) = \frac{3}{2}\,NkT + N\,\varphi(V,\eta) \quad ,$$

$$P(V,T) = \frac{NkT}{V} - N\left[\frac{\partial\,\varphi(V,\eta)}{\partial V}\right]_{\eta} \quad . \qquad (26)$$

The function $\alpha(\eta)$ is given by

$$\alpha(\eta) = 2.2955\,\ln\,(1-\eta) + 5.2574\,\eta\sum_{k=0}^{3} b_k\left(\frac{\eta}{1-\eta}\right)^k \quad , \qquad (27)$$

where b_0 = 1, b_1 = .73977, b_2 = -.12148, and b_3 = .01243. The function $\varphi(V,\eta)$ is given by

$$\varphi(V,\eta) = \frac{g(\eta)}{2\eta}\int_1^{X_M} e^{-c(x-1)}\,\varepsilon(V_s,V)\,\frac{dx}{x} \quad ,$$

$$c = 3.2285\,\eta/(1-\eta) \quad ,$$

$$\frac{1}{2}\,g(\eta)\int_1^{X_M} e^{-c(x-1)}\,\frac{dx}{x} = 1 \quad ,$$

$$g(\eta) = 2.9619\,\eta\sum_{k=1}^{4} A_k\left(\frac{\eta}{1-\eta}\right)^k \quad , \qquad (28)$$

where A_0 = 1, A_1 = 1.8512, A_2 =.66621, A_3 = - .343, and A_4 = .0662. $\varepsilon(V_s,V)$ is the energy of an atom in the solid at a specific volume, $V_s = \eta V x^3$, when a fraction $(V-V_s)/V$ of the sites are vacant.

In this report we use a slightly modified expression for $\epsilon(V_s,V)$. Let $E_c(V_s)$ be the energy of the solid at a volume V_s, when no vacancies are present. If a fraction, f, of the atoms are removed, each atom has only 1-f of the bonds it had originally. Hence the energy is

$$\epsilon(V_s,V) \cong (1-f)\ E_c(V_s) = \frac{V_s}{V}\ E_c(V_s). \tag{29}$$

Equation (29) was used successfully in our previous report. At very high densities, however, this expression must be modified. Note that, as $V \to 0$,

$$E_c(V) \to E_F(V) = \frac{3Nh^2}{10m}\left(\frac{3N}{8\pi V}\right)^{2/3}, \tag{30}$$

where $E_F(V)$ is the Fermi energy of a system of free electrons (see the appendix). According to Eq. (29), $\epsilon(V_s,V) \to 0$ as $V_s \to 0$. A more realistic expression at high densities is

$$\epsilon(V_s,V) \cong \left(\frac{V_s}{V}\right)^{2/3} E_c(V_s). \tag{31}$$

According to Eqs. (30) and (31), $\epsilon(V_s,V) \to E_F(V)$ as $V_s \to 0$. In other words, when the lattice is tightly packed, the electrons are delocalized and the energy approaches the limit of a system of free electrons. To interpolate between the high- and low-density cases, we propose the following expression.

$$\epsilon(V_s,V) = \left\{\beta(V_s)\left(\frac{V_s}{V}\right)^{2/3} + [1 - \beta(V_s)]\ \frac{V_s}{V}\right\} E_c(V_s)\ , \tag{32}$$

where $\beta(V_s)$ is the fraction of electrons which are delocalized, or "free." A very crude estimate of $\beta(V_s)$ can be obtained in the following manner. We note that the Thomas-Fermi-Dirac (TFD) pressure for hydrogen can be fit by[24]

$$P_{TFD}(V) = \frac{2}{3}\ \frac{E_F(V)}{V}\ e^{-\ 0.9862V^{1/3}}\ ,$$

where V has units of cm^3/g-mole. Hence we take

$$\beta(V_s) \cong e^{-.9862\ V_s^{1/3}}\ , \tag{33}$$

to be the fraction of "free" electrons in the system.

This alteration to the theory does not change any of the results which we discussed in our previous report, but it has a significant effect at very high densities. As $V \to 0$, we find that the Helmholtz free energy, internal energy, and pressure approach the following formulas.

$$\begin{aligned} A(V,T) &\to A_o(V,T) + E_F(V), \\ E(V,T) &\to \frac{3}{2}\ NkT + E_F(V), \\ P(V,T) &\to \frac{NkT}{V} + \frac{2}{3}\ \frac{E_F(V)}{V}\ . \end{aligned} \tag{34}$$

Equation (34) describes an ideal gas of nuclei moving in a uniform electron "sea". Hence our modification to the theory provides a reasonable interpolation to the correct high-density limit.

The translational contributions to the thermodynamic properties of the molecular fluid are calculated with the CRIS model, as described above, using the zero-temperature isotherm given in Eq. (2). The vibration-rotation terms are calculated as described in Section VI. For the atomic fluid we use the zero-temperature isotherm for the metallic solid (without zero-point energy), defined by Eq. (11) and parameters given in Table I. The electronic contributions are calculated as discussed in Section VII. The equations of state for the two pure fluids are combined as described in Section IV.

VI. MOLECULAR VIBRATION AND ROTATION

At low densities, the vibrational-rotational contributions to the equation of state can be calculated in a straightforward manner. The partition function for a diatomic molecule is[25]

$$Q_{VR} = \frac{1}{\sigma} \sum_{n=0}^{n_M} \sum_{J=0}^{J_M} (2J + 1)\, e^{-E(n,J)/kT} \quad , \qquad (35)$$

where the sum is taken over the vibrational quantum numbers, n, and the rotational quantum numbers, J, and σ is the symmetry number ($\sigma = 1$ for heteronuclear molecules, $\sigma = 2$ for homonuclear molecules). To a good approximation, the energy levels, E(n,J), are given by

$$\frac{E(n,J)}{hc} = W_e(n + \tfrac{1}{2}) + B_e\, J(J + 1) - W_eX_e(n + \tfrac{1}{2})^2$$
$$- D_eJ^2(J + 1)^2 - \alpha_e(n + \tfrac{1}{2})\, J(J + 1). \qquad (36)$$

W_e is the vibrational frequency, and B_e is the rotational constant. The last three terms represent effects due to anharmonicity, centrifugal distortion, and vibration-rotation coupling. For most molecules, the stretching potential can be represented by the Morse formula,

$$U_o(R) = D_o \left[e^{-S(R-R_o)} - 1 \right]^2 , \qquad (37)$$

where D_o is the dissociation energy, and R_o is the equilibrium nuclear distance of the molecule. For deuterium, $D_o = 5.5103 \times 10^4$ °K, $R_o = 0.74141$ Å, and $S = 1.94596$ Å^{-1}. For a Morse potential, it can be shown that[26]

$$W_e = \frac{S}{2\pi C} \sqrt{\frac{2D_o}{\mu}} \; ,$$
$$B_e = \frac{h}{8\pi^2 \mu R_o{}^2 C} \; ,$$
$$W_eX_e = \frac{hcW_e{}^2}{4D_o} \; ,$$
$$D_e = \frac{4B_e{}^3}{W_e{}^2} \; ,$$
$$\alpha_e = 3B_e\sqrt{\frac{hcB_e}{D_o}} \left(1 - \sqrt{\frac{B_e}{W_eX_e}} \right). \qquad (38)$$

μ is the reduced mass of the molecule.

The highest allowed vibrational quamtum number, n_M, is given by

$$n_M \le \frac{W_e}{2W_eX_e} - \frac{1}{2} < n_M + 1. \qquad (39)$$

For a given vibrational quantum number, n, the highest allowed rotational quantum number, $J_M(n)$, is

$$J_M \le \frac{1}{2} \left[\sqrt{1 + 2\, \frac{1 - \alpha_e(n + 1/2)}{De}} - 1 \right] < J_M + 1. \qquad (40)$$

At high densities, the molecular potential function and the energy levels, E(n,J), are perturbed by the forces of neighboring molecules. In this work we ignore the effect of hindered rotation, which is important only at low temperatures. The potential is of the form

$$U(R) = U_o(R) + U_1(R) \quad , \qquad (41)$$

where $U_o(R)$ is the potential of the free molecule, Eq. (37), and $U_1(R)$ is the contribution from neighboring molecules. To calculate $U_1(R)$, we assume that the molecule is surrounded by 12 nearest neighbors, smeared out over a spherical shell of radius $a = 2^{1/6}(V/N)^{1/3}$. The molecule is assumed to vibrate with its center of mass fixed at the center of this sphere. The geometry is shown in Fig. 3. Let $\phi_A(r)$ be the potential between a deuterium <u>atom</u> and a nearest neighbor molecule. Averaging over all the nearest neighbors, as was done in the LJD theory, Section II, we find

$$U_1(R) = 6 \int_{-1}^{1} 2\, \phi_A(r)\, d\cos\theta \cong 6 \int_{-1}^{1} \phi(r)\, d\cos\theta \; ,$$
$$r = \sqrt{R^2/4 - Ra\cos\theta + a^2} \; , \qquad (42)$$

where $\phi(r)$ is the potential between two molecules. Substituting for $\phi(r)$ from Eq. (6), we obtain the following result.

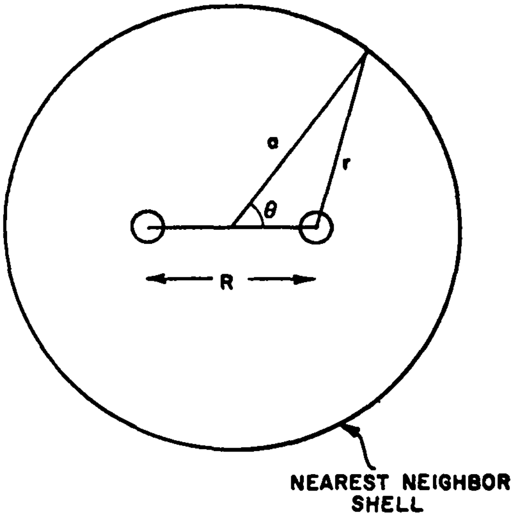

Fig. 3. Geometry of a vibrating molecule surrounded by nearest neighbors. The symbols are the same as those used in Eq. (42).

$$U_1(R) = C_1 \frac{\sinh(C_2R)}{R} - C_3 \cosh(C_2R)$$

$$- C_4 \frac{\sinh(C_5R)}{R} + C_6 \cosh(C_5R) \ , \qquad (43)$$

where

$$C_1 = 12\epsilon \exp[B(1 - A/\sigma)]\, 2\sigma\, (1 + \sigma/BA)/B \ ,$$

$$C_2 = B/2\sigma \ ,$$

$$C_3 = 12\epsilon \exp[B(1 - A/\sigma)]\, \sigma/BA \ ,$$

$$C_4 = 12\epsilon \exp[C(1 - A/\sigma)]\, 2\sigma\, (1 + \sigma/CA)/C \ ,$$

$$C_5 = C/2\sigma \ ,$$

$$C_6 = 12\epsilon \exp[C(1 - A/\sigma)]\, \sigma/CA \ .$$

Having determined the potential U(R) as a function of specific volume, we calculate the equilibrium nuclear distance, R_e; vibrational frequency, W_e; and rotational constant, B_e, as follows.

$$\left(\frac{dU(R)}{dR}\right)_{R=R_e} = 0 \ ,$$

$$W_e = \frac{1}{2\pi C}\sqrt{\frac{1}{\mu}\left(\frac{d^2U}{dR^2}\right)_{R_e}} \ ,$$

$$B_e = \frac{h}{8\pi^2 \mu R_e^2 C} \ . \qquad (44)$$

For simplicity, we assume that the dissociation energy, D_o, is independent of density, so that W_eX_e, D_e, and α_e can be calculated according to Eq. (38). Our considerations imply that the perturbed Morse potential for the molecule is

$$U(R) = D_o\left[e^{-S'(R-R_e)} - 1\right]^2 \ , \qquad (45)$$

$$S' = 2\pi C\, W_e \sqrt{\mu/2D_o} \ .$$

Another phenomenon that arises as the density increases is that the metallic state becomes more stable relative to the molecular state. A schematic illustration of the potential is shown in Fig. 4. For sufficiently small displacements of the internuclear distance, R, the molecule stays within its

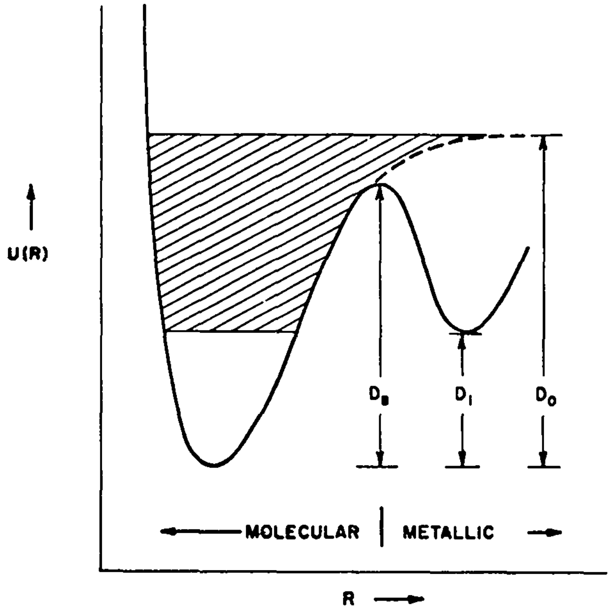

Fig. 4. Schematic illustration of the molecular potential function at a high density.

potential well. For large R, it can "tunnel" through the barrier, D_B, and go into the more stable metallic state, accompanied by changes in its translational and electronic degrees of freedom Let D_i be the difference in energy between the molecular and metallic states. At low densities, $D_i = D_B = D_o$, and all energy levels in the potential well are stable. At high densities, all energy levels with energies greater than D_i (shaded region in Fig. 4) are "unstable" because they can give rise to a metallic transition.

From a quantum-mechanical point of view, it is incorrect to speak of independent "molecular" and "metallic" states of the system; the true wave function has properties of both states. To solve the problem rigorously, it would be necessary to do a detailed calculation, including coupling between translational and vibrational motions. Such a calculation is beyond the scope of this report.

A more straightforward approach is to exclude from the partition function, Q_{VR}, all energy levels with energies greater than D_i. However, such a procedure results in a discontinuous change in Q_{VR} whenever a level crosses into the shaded region of Fig. 4. Consequently, we use the following approach. The partition function is assumed to be

$$Q_{VR} = \frac{1}{\sigma} \sum_n \sum_J (2J+1)\ F(n,J) E^{-E(n,J)/kT} \quad , \qquad (46)$$

where F(n,J) is a "weighting factor." We require that $F(n,J) = 1$ for $E(n,J) \leq D_i$, and $F(n,J) = 0$ for $E(n,J) \geq D_B$. Assuming that F(n,J) is a linear function of energy,

$$F(n,J) = \frac{D_B - E(n,J)}{D_B - D_i} \quad . \qquad (47)$$

We take D_B to be the value of the stretching potential, U(R), when R is equal to the nearest-neighbor distance between atoms in the metallic lattice. Hence,

$$D_B = U \left[2^{1/6} (V/2N)^{1/3} \right] , \qquad (48)$$

where U(R) is given by Eq. (45). The above procedure is very crude, but it gives the correct qualitative behavior in the region of transition from the molecular to the metallic state.

Finally, we note that the vibrational-rotational contributions to the thermodynamic quantities are given by the following formulas.

$$A_{VR}(V,T) = - NkT \ln Q_{VR}(V,T) \quad ,$$

$$E_{VR}(V,T) = NkT^2 \left(\frac{\partial \ln Q_{VR}}{\partial T} \right)_V \quad ,$$

$$P_{VR}(V,T) = NkT \left(\frac{\partial \ln Q_{VR}}{\partial V} \right)_T \quad . \qquad (49)$$

Derivatives of $\ln Q_{VR}$ are calculated numerically.

VII. EXCITED ELECTRONIC STATES AND IONIZATION

The contribution of excited electronic states and ionization to the thermodynamic properties of atomic deuterium can be calculated from either one of two theories - the Saha theory of ionization equilibrium,[23] which is valid at low densities, or the Thomas-Fermi-Dirac (TFD) theory,[24] which is valid at high densities. Unfortunately, there exists an intermediate density range where neither theory is realistic. In this section, however, we show how the Saha theory can be modified so that it is forced to agree with the TFD results at high densities and provides a reasonable interpolation in between.

In order to derive an expression for the electronic partition function, we first consider the ideal gas limit. If there are N_A atoms, N_p deuterons, and N_e electrons, the total partition function is given by[23]

$$Q(V,T) = \frac{1}{N_A! N_p! N_e!} \left[V \left(\frac{2\pi M_A kT}{h^2} \right)^{3/2} q_A \right]^{N_A} \times$$
$$\left[V \left(\frac{2\pi M_p kT}{h^2} \right)^{3/2} \right]^{N_p} \left[2V \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} e^{-I/kT} \right]^{N_e} , \qquad (50)$$

where M_A, M_p, and M_e are the atom, deuteron, and electron masses, respectively, and I is the ionization energy (13.6eV). q_A is the atomic partition function (sum over bound electronic states of the atom). The factor of 2 in the last term arises from spin degeneracy of the free electron. We note that $N_p = N_e$, and $N_p + N_A = N$, where N is the total number of atoms present before ionization. Taking $M_A = M_p$, the partition function can be written as a product of a translational and an electronic term,

$$Q = Q_t Q_e \ . \tag{51}$$

Q_t is the translational partition function for an ideal gas,

$$Q_t(V,T) = \left[\frac{eV}{N} \left(\frac{2\pi M_A kT}{h^2} \right)^{3/2} \right]^N \ . \tag{52}$$

Defining f to be the fraction of atoms that are ionized, we have $N_p = N_e = fN$, $N_A = (1-f)N$. The electronic partition function can be written

$$Q_e(V,T) = \frac{1}{f^{2fN}(1-f)^{(1-f)N}} \, q_A^{(1-f)N} \, q_e^{fN} \, e^{-fNI/kT} \ , \tag{53}$$

where q_e is the partition function for a free electron.

$$q_e = \frac{2eV}{N} \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} \ . \tag{54}$$

In this work, we assume that the translational and electronic contributions to the equations of state are separable, so that Eq. (53) is valid even when we are dealing with imperfect gases. Since the electronic terms are significant only at high temperatures, where the translational motion approaches ideal gas behavior, this approximation seems reasonable.

The electronic contribution to the free energy is

$$\begin{aligned} A_e &= -kT \ln Q_e \\ &= NkT \Big\{ 2f \ln f + (1-f) \ln(1-f) \\ &\quad - (1-f) \ln q_a - f \ln q_e + f \frac{I}{kT} \Big\} \ . \end{aligned} \tag{55}$$

To determine f, the dissociation fraction, we minimize the free energy. The result is

$$\frac{1-f}{f^2} \, \frac{q_e e^{-I/kT}}{e q_A} = 1 \ . \tag{56}$$

Finally, the electronic contributions to the energy and pressure are given by

$$E_e = NkT^2 \left[(1-f) \left(\frac{\partial \ln q_A}{\partial T} \right)_V + f \left(\frac{\partial \ln q_e}{\partial T} \right)_V \right] + NfI \ , \tag{57}$$

and

$$\begin{aligned} P_e = NkT &\left[(1-f) \left(\frac{\partial \ln q_A}{\partial V} \right)_T + f \left(\frac{\partial \ln q_e}{\partial V} \right)_T \right] \\ &- Nf \, dI/dV \ . \end{aligned} \tag{58}$$

In the classical case, q_A and I do not depend upon volume and make no contribution to the pressure. However, these terms will be important in our "modified" Saha theory.

The electronic partition function for the atom is given by

$$q_A = \sum_{n=1} g_n e^{-\epsilon_n/kT} \ , \tag{59}$$

where ϵ_n, the energy of the n-th level, is

$$\epsilon_n = 13.6 \left(1 - \frac{1}{n^2}\right) \ ,$$

and the degeneracy factor is $g_n = 2n^2$. Because hydrogen has an infinite number of bound electronic states, the sum must be cut off at some value to make q_A finite. It is usually argued that the highest energy levels, for which the radius of the Bohr orbit is greater than the radius of a Wigner-Seitz cell, are broadened into the ionization continuum and should not be included in the sum. Hence the nth level is cut off if

$$n^2 a_o \geq \left(\frac{3}{4\pi}\frac{V}{N}\right)^{1/3}$$

where a_o is the Bohr radius (.5292 Å). By this reasoning, the n=2 level should not be "counted" at densities greater than .03 g/cm^3. At lower densities, our numerical comparisons show that the excited states make very little contribution to any of the thermodynamic properties, because ionization occurs before these levels become populated. Consequently, we ignore excited states and take $q_A = 2$ in this work.

The Saha and TFD predictions of the electronic contributions to the pressure, free energy and internal energy are shown in Figs. 5 to 7. TFD data were obtained from R. D. Cowan.[24] Notice that the two sets of data agree fairly well with one another for temperatures above 5 eV.

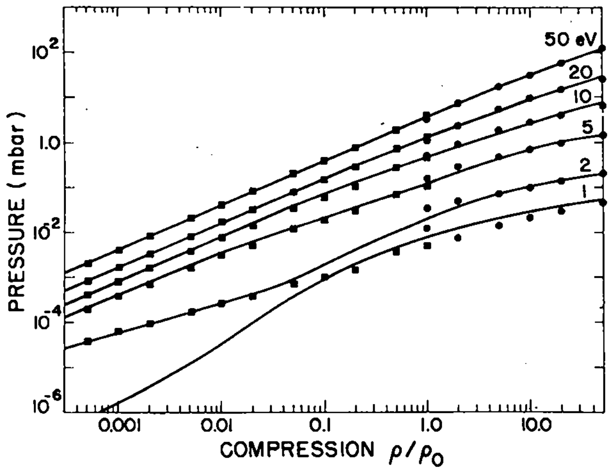

Fig. 5. Thermal electronic contributions to the pressure. Squares are Saha calculations. Circles are TFD calculations. The lines are our modified Saha theory.

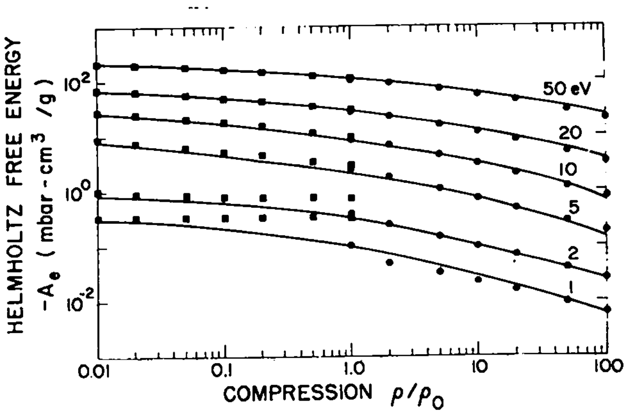

Fig. 6. Thermal electronic contributions to the Helmholtz free energy. Symbols used are defined in the caption of Fig. 5.

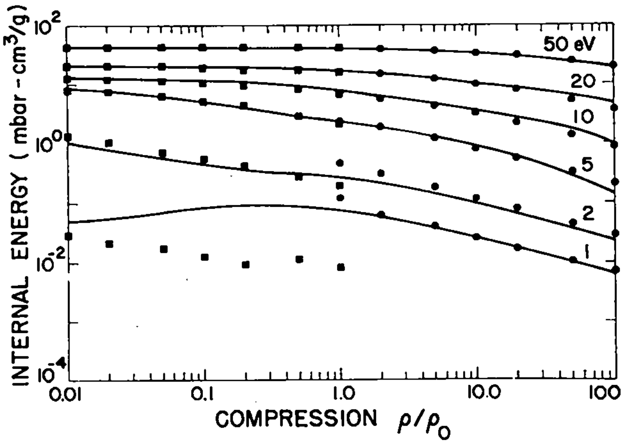

Fig. 7. Thermal electronic contributions to the internal energy. Symbols used are defined in the caption of Fig. 5.

At high densities, the Saha theory discussed above has two major defects. First, the free electron partition function, defined by Eq. (54), does not include the quantum-mechanical effects which follow from Fermi-Dirac statistics. Second, the bound electronic states of the atom are treated as discrete levels. At high densities these levels are broadened into bands, with the electrons obeying quantum statistics.

In the appendix, we derive expressions for the thermodynamic properties of a uniform electron gas obeying Fermi-Dirac statistics. The free-electron partition function is shown to be

$$q_e(V,T) = \left[\frac{1 + by + .2636y^2}{.2636y^2}\right]^{3/4} ,$$

$$y = \frac{h^2}{2\pi m_e kT}\left(\frac{N}{2V}\right)^{2/3} . \qquad (60)$$

For a uniform gas, b = .7173. However we find that b = .4242 gives a better fit to the TFD data, possibly because of exchange effects. The ionization energy should also be modified to include zero-point energy of the electrons.

$$I = 13.6 \text{ eV} + \frac{3h^2}{10m_e}\left(\frac{3N}{8\pi V}\right)^{2/3} . \qquad (61)$$

Finally, we must modify the atomic partition function so that it approaches the electron gas result at high densities. As $V \to 0$, $y \to \infty$, we note that

$$\ln q_e \to \frac{3}{4}\ln\left(1 + \frac{b}{.2636y}\right) \to \frac{1}{\frac{4}{3}\frac{.2636}{b}y} .$$

We assume that

$$\ln q_A = \frac{\ln 2}{1 + \frac{4}{3}\frac{.2636 \ln 2}{b}y} . \qquad (62)$$

Equation (62) can be interpreted as follows. Interaction between the atoms splits the 2N ground electronic states into a 2N-fold degenerate band of levels. At low densities this band is very narrow, so that all the energy levels can be populated, even at low temperatures. Hence $q_A = 2$. At high densities the band widens, and only the bottom half of the levels can be populated at low temperatures. Hence $q_A \to 1$ as $V \to 0$, $T \to 0$. Eq. (62) provides a reasonable interpolation between these two extremes.

With these new definitions of q_e, I, and q_A, the Saha calculations can be carried out as previously described. The results are shown in Figs. 5 to 7. Our modified theory agrees very well with the TFD data at high densities and provides a reasonable approximation at lower densities. It should be noted that the molecules are only partially dissociated at low temperatures, and that the electronic contributions are small compared to the translational contributions. Hence the errors in our treatment are minimized.

VIII. PHASE DIAGRAM

Using the methods discussed in previous sections, thermodynamic properties for each of the three phases, molecular solid, metallic solid, and fluid, can be calculated. In this section we use the results to construct the phase diagram for deuterium. The diagrams for hydrogen and tritium should be similar, but isotope effects may cause shifts in the phase lines.

According to thermodynamics, the phase that is stable at a given pressure and temperature is the one having the lowest Gibb's free energy, F = A + PV. The coexistence line between two phases is determined by finding the pressure and temperature at which the two phases have equal free energies. Consider phases a and b at a temperature T. Assume that phase a is stable at low pressures and phase b is stable at high pressures. The coexistence line is defined by the relations

$$P_a(V_a,T) = P_b(V_b,T) \ , \quad F_a(V_a,T) = F_b(V_b,T) \ , \qquad (63)$$

which we solve for V_a and V_b by an iterative method. For $V > V_a$, phase a is stable; for $V < V_b$, phase b is stable. For $V_b < V < V_a$, a mixture of the two phases exists. The internal energy and Helmholtz free energy of the mixture are given by

$$E(V,T) = \frac{V_b - V}{V_b - V_a} E_a(V_a,T) + \frac{V - V_a}{V_b - V_a} E_b(V_b,T) ,$$

$$A(V,T) = \frac{V_b - V}{V_b - V_a} A_a(V_a,T) + \frac{V - V_a}{V_b - V_a} A_b(V_b,T) . \qquad (64)$$

Our calculated phase diagram is shown in Fig. 8. Specific volumes on the phase lines are shown

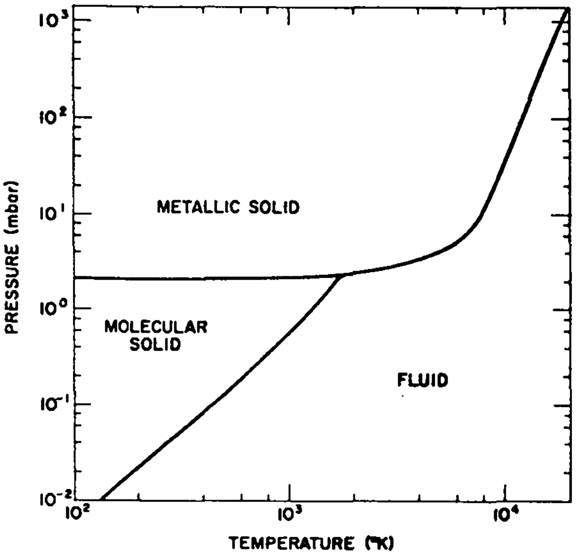

Fig. 8. Phase diagram for deuterium.

in Fig. 9. The transition from a molecular solid to a metallic solid occurs at 2.2-2.3 mbar, nearly independent of temperature. The melting pressure of the molecular solid increases with the temperature. At 1679°K and 2.3 mbar, these two phase lines cross. This temperature and pressure specify a triple point, where all three phases coexist. At temperatures above 1679°K, the molecular solid is no longer stable and there is a melting curve for the metallic solid. At high temperatures we find that the changes in volume and the thermodynamic quantities are very small, on melting, but are finite. In other words, no solid-fluid critical point is reached. For temperatures above 14,000°K, the specific volumes on melting can be fit to the approximate formulas

$$V(\text{fluid}) = (8212.7/T)^{2.8} \text{ cm}^3/\text{mole},$$

$$V(\text{solid}) = .9872 \; V(\text{fluid}).$$

IX. RESULTS

The pressure, internal energy, and Helmholtz free energy for deuterium are given as functions of compression and temperature in Table II. The compression, η, is defined in terms of the density, ρ, by $\eta = \rho/\rho_0$, where $\rho_0 = .17$ g/cm^3. The last column in Table II specifies the phase. For the gas phase, the fraction of dissociation, f, is also presented. A more detailed equation-of-state table

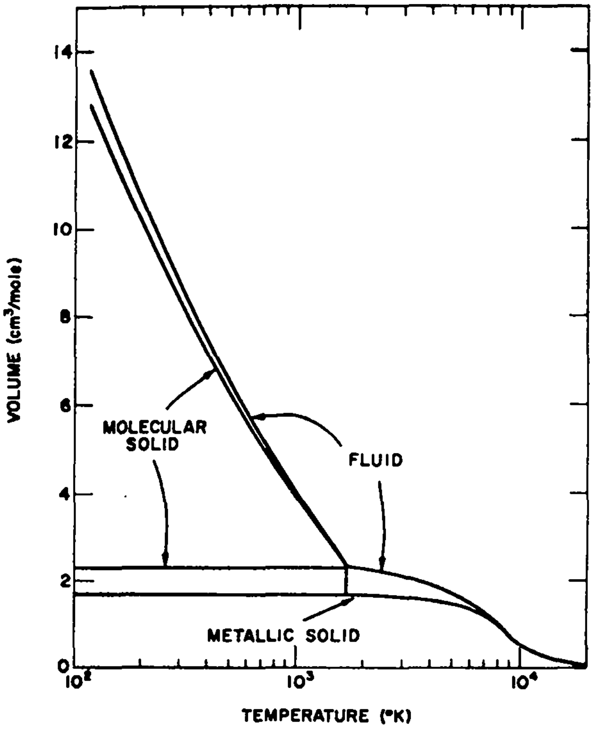

Fig. 9. Specific volumes on the phase lines.

is presently in use at this Laboratory.

In Figs. 10 and 11, the pressure and internal energy on several isotherms are shown. The experimental data of Michels et al.[27] are given in Fig. 10. For completeness, the 0°K isotherm is also shown. The effect of phase transitions on the equation of state can be observed more readily in the figures.

X. CONCLUSIONS

We have described a theoretical equation of state for deuterium, suitable for use over a wide range of temperatures and densities. In such a comprehensive study, it has been necessary to make numerous approximations. Consequently, there are many uncertainties in our work. However, we have tried to consider all of the problems peculiar to deuterium and to treat the physics with as much accuracy as is feasible with current theoretical methods.

TABLE II. DEUTERIUM EQUATION OF STATE.

TEMPERATURE = 1.7783E+02 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	6.2854E-07	8.9332E-03	-5.0344E-02	FLUID, F = 1.8381E-63
1.7783E-03	1.1180E-06	8.9309E-03	-4.8216E-02	FLUID, F = 1.3294E-63
3.1623E-03	1.9892E-06	8.9270E-03	-4.6086E-02	FLUID, F = 9.8311E-64
5.6234E-03	3.5407E-06	8.9206E-03	-4.3955E-02	FLUID, F = 7.5100E-64
1.0000E-02	6.3077E-06	8.9097E-03	-4.1821E-02	FLUID, F = 6.0138E-64
1.7783E-02	1.1254E-05	8.8912E-03	-3.9682E-02	FLUID, F = 5.1718E-64
3.1623E-02	2.0138E-05	8.8596E-03	-3.7533E-02	FLUID, F = 4.9822E-64
5.6234E-02	3.6235E-05	8.8054E-03	-3.5366E-02	FLUID, F = 5.7908E-64
1.0000E-01	6.5947E-05	8.7122E-03	-3.3161E-02	FLUID, F = 9.2574E-64
1.7783E-01	1.2302E-04	8.5527E-03	-3.0881E-02	FLUID, F = 2.5651E-63
3.1623E-01	2.4330E-04	8.2863E-03	-2.8427E-02	FLUID, F = 1.8570E-62
5.6234E-01	5.5837E-04	7.8698E-03	-2.5515E-02	FLUID, F = 7.3439E-61
1.0000E+00	1.8440E-03	7.7303E-03	-2.1054E-02	FLUID, F = 6.2287E-58
1.7783E+00	1.0537E-02	1.1851E-02	-9.6531E-03	FLUID, F = 1.2594E-52
3.1623E+00	6.5030E-02	3.5845E-02	2.8441E-02	MOLECULAR SOLID
5.6234E+00	4.1981E-01	1.7242E-01	1.7399E-01	MOLECULAR SOLID
1.0000E+01	2.0249E+00	6.0828E-01	6.1738E-01	MOLECULAR SOLID
1.7783E+01	4.1658E+00	1.2451E+00	1.2450E+00	METALLIC SOLID
3.1623E+01	1.7183E+01	2.5129E+00	2.5128E+00	METALLIC SOLID
5.6234E+01	5.9926E+01	5.1643E+00	5.1642E+00	METALLIC SOLID
1.0000E+02	1.9057E+02	1.0087E+01	1.0087E+01	METALLIC SOLID
1.7783E+02	5.7251E+02	1.8602E+01	1.8602E+01	METALLIC SOLID
3.1623E+02	1.6569E+03	3.2683E+01	3.2683E+01	METALLIC SOLID
5.6234E+02	4.6749E+03	5.5270E+01	5.5270E+01	METALLIC SOLID
1.0000E+03	1.2954E+04	9.0743E+01	9.0743E+01	METALLIC SOLID

TEMPERATURE = 3.1623E+02 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	1.1181E-06	1.6153E-02	-9.8754E-02	FLUID, F = 4.0566E-35
1.7783E-03	1.9893E-06	1.6151E-02	-9.4967E-02	FLUID, F = 2.8858E-35
3.1623E-03	3.5406E-06	1.6148E-02	-9.1178E-02	FLUID, F = 2.0755E-35
5.6234E-03	6.3062E-06	1.6143E-02	-8.7384E-02	FLUID, F = 1.5227E-35
1.0000E-02	1.1246E-05	1.6135E-02	-8.3582E-02	FLUID, F = 1.1517E-35
1.7783E-02	2.0101E-05	1.6120E-02	-7.9765E-02	FLUID, F = 9.1146E-36
3.1623E-02	3.6076E-05	1.6097E-02	-7.5921E-02	FLUID, F = 7.7292E-36
5.6234E-02	6.5238E-05	1.6058E-02	-7.2029E-02	FLUID, F = 7.3177E-36
1.0000E-01	1.1967E-04	1.5994E-02	-6.8045E-02	FLUID, F = 8.3164E-36
1.7783E-01	2.2580E-04	1.5892E-02	-6.3884E-02	FLUID, F = 1.2899E-35
3.1623E-01	4.5150E-04	1.5750E-02	-5.9353E-02	FLUID, F = 3.4288E-35
5.6234E-01	1.0239E-03	1.5646E-02	-5.3962E-02	FLUID, F = 2.3458E-34
1.0000E+00	3.0373E-03	1.6240E-02	-4.6153E-02	FLUID, F = 8.6029E-33
1.7783E+00	1.3823E-02	2.2142E-02	-2.9684E-02	FLUID, F = 5.8726E-30
3.1623E+00	7.1982E-02	4.7079E-02	1.9128E-02	MOLECULAR SOLID
5.6234E+00	4.3037E-01	1.8390E-01	1.7159E-01	MOLECULAR SOLID
1.0000E+01	2.0407E+00	6.1979E-01	6.2083E-01	MOLECULAR SOLID
1.7783E+01	4.1674E+00	1.2457E+00	1.2447E+00	METALLIC SOLID
3.1623E+01	1.7184E+01	2.5130E+00	2.5128E+00	METALLIC SOLID
5.6234E+01	5.9926E+01	5.1643E+00	5.1642E+00	METALLIC SOLID
1.0000E+02	1.9057E+02	1.0087E+01	1.0087E+01	METALLIC SOLID
1.7783E+02	5.7251E+02	1.8602E+01	1.8602E+01	METALLIC SOLID
3.1623E+02	1.6569E+03	3.2683E+01	3.2683E+01	METALLIC SOLID
5.6234E+02	4.6749E+03	5.5270E+01	5.5270E+01	METALLIC SOLID
1.0000E+03	1.2954E+04	9.0743E+01	9.0743E+01	METALLIC SOLID

TABLE II. CONTINUED.

TEMPERATURE = 5.6234E+02 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	1.9886E-06	2.9066E-02	-1.9224E-01	FLUID, F = 3.8975E-19
1.7783E-03	3.5383E-06	2.9065E-02	-1.8551E-01	FLUID, F = 2.7678E-19
3.1623E-03	6.2986E-06	2.9064E-02	-1.7877E-01	FLUID, F = 1.9667E-19
5.6234E-03	1.1221E-05	2.9061E-02	-1.7202E-01	FLUID, F = 1.4087E-19
1.0000E-02	2.0018E-05	2.9057E-02	-1.6525E-01	FLUID, F = 1.0266E-19
1.7783E-02	3.5801E-05	2.9051E-02	-1.5846E-01	FLUID, F = 7.6965E-20
3.1623E-02	6.4313E-05	2.9042E-02	-1.5161E-01	FLUID, F = 6.0265E-20
5.6234E-02	1.1646E-04	2.9030E-02	-1.4466E-01	FLUID, F = 5.0458E-20
1.0000E-01	2.1401E-04	2.9017E-02	-1.3755E-01	FLUID, F = 4.7018E-20
1.7783E-01	4.0425E-04	2.9016E-02	-1.3010E-01	FLUID, F = 5.2317E-20
3.1623E-01	8.0529E-04	2.9077E-02	-1.2200E-01	FLUID, F = 7.8738E-20
5.6234E-01	1.7826E-03	2.9417E-02	-1.1247E-01	FLUID, F = 1.9990E-19
1.0000E+00	4.8540E-03	3.1053E-02	-9.9395E-02	FLUID, F = 1.2635E-18
1.7783E+00	1.8516E-02	3.9278E-02	-7.5480E-02	FLUID, F = 3.7887E-17
3.1623E+00	9.4153E-02	7.8805E-02	-1.3833E-02	FLUID, F = 1.2388E-14
5.6234E+00	4.4896E-01	2.0428E-01	1.5558E-01	MOLECULAR SOLID
1.0000E+01	2.0686E+00	6.4028E-01	6.1518E-01	MOLECULAR SOLID
1.7783E+01	4.1815E+00	1.2507E+00	1.2428E+00	METALLIC SOLID
3.1623E+01	1.7190E+01	2.5144E+00	2.5123E+00	METALLIC SOLID
5.6234E+01	5.9929E+01	5.1646E+00	5.1641E+00	METALLIC SOLID
1.0000E+02	1.9057E+02	1.0087E+01	1.0087E+01	METALLIC SOLID
1.7783E+02	5.7251E+02	1.8602E+01	1.8602E+01	METALLIC SOLID
3.1623E+02	1.6569E+03	3.2683E+01	3.2683E+01	METALLIC SOLID
5.6234E+02	4.6749E+03	5.5270E+01	5.5270E+01	METALLIC SOLID
1.0000E+03	1.2954E+04	9.0743E+01	9.0743E+01	METALLIC SOLID

TEMPERATURE = 1.0000E+03 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	3.5364E-06	5.3230E-02	-3.7197E-01	FLUID, F = 4.0999E-10
1.7783E-03	6.2924E-06	5.3230E-02	-3.5999E-01	FLUID, F = 2.9373E-10
3.1623E-03	1.1201E-05	5.3231E-02	-3.4800E-01	FLUID, F = 2.0914E-10
5.6234E-03	1.9955E-05	5.3233E-02	-3.3600E-01	FLUID, F = 1.4865E-10
1.0000E-02	3.5600E-05	5.3236E-02	-3.2396E-01	FLUID, F = 1.0620E-10
1.7783E-02	6.3663E-05	5.3244E-02	-3.1188E-01	FLUID, F = 7.6972E-11
3.1623E-02	1.1434E-04	5.3261E-02	-2.9970E-01	FLUID, F = 5.7251E-11
5.6234E-02	2.0693E-04	5.3296E-02	-2.8736E-01	FLUID, F = 4.4376E-11
1.0000E-01	3.7971E-04	5.3370E-02	-2.7472E-01	FLUID, F = 3.6687E-11
1.7783E-01	7.1448E-04	5.3533E-02	-2.6153E-01	FLUID, F = 3.3623E-11
3.1623E-01	1.4085E-03	5.3918E-02	-2.4727E-01	FLUID, F = 3.6533E-11
5.6234E-01	3.0306E-03	5.4927E-02	-2.3082E-01	FLUID, F = 5.2941E-11
1.0000E+00	7.6753E-03	5.8013E-02	-2.0931E-01	FLUID, F = 1.2546E-10
1.7783E+00	2.5387E-02	6.9287E-02	-1.7421E-01	FLUID, F = 6.7962E-10
3.1623E+00	1.1076E-01	1.1430E-01	-9.7208E-02	FLUID, F = 1.3593E-08
5.6234E+00	5.2116E-01	2.7408E-01	1.0422E-01	FLUID, F = 1.9970E-06
1.0000E+01	2.1190E+00	6.7703E-01	5.8411E-01	MOLECULAR SOLID
1.7783E+01	4.2513E+00	1.2759E+00	1.2299E+00	METALLIC SOLID
3.1623E+01	1.7237E+01	2.5251E+00	2.5082E+00	METALLIC SOLID
5.6234E+01	5.9954E+01	5.1680E+00	5.1629E+00	METALLIC SOLID
1.0000E+02	1.9059E+02	1.0088E+01	1.0086E+01	METALLIC SOLID
1.7783E+02	5.7251E+02	1.8602E+01	1.8602E+01	METALLIC SOLID
3.1623E+02	1.6569E+03	3.2683E+01	3.2683E+01	METALLIC SOLID
5.6234E+02	4.6749E+03	5.5270E+01	5.5270E+01	METALLIC SOLID
1.0000E+03	1.2954E+04	9.0743E+01	9.0743E+01	METALLIC SOLID

TABLE II. CONTINUED.

TEMPERATURE = 1.7783E+03 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	6.2889E-06	1.0209E-01	-7.1785E-01	FLUID, F = 5.0289E-05
1.7783E-03	1.1189E-05	1.0208E-01	-6.9655E-01	FLUID, F = 3.6484E-05
3.1623E-03	1.9917E-05	1.0207E-01	-6.7523E-01	FLUID, F = 2.6253E-05
5.6234E-03	3.5479E-05	1.0207E-01	-6.5389E-01	FLUID, F = 1.8758E-05
1.0000E-02	6.3279E-05	1.0208E-01	-6.3250E-01	FLUID, F = 1.3353E-05
1.7783E-02	1.1311E-04	1.0211E-01	-6.1102E-01	FLUID, F = 9.5283E-06
3.1623E-02	2.0299E-04	1.0216E-01	-5.8939E-01	FLUID, F = 6.8761E-06
5.6234E-02	3.6680E-04	1.0227E-01	-5.6750E-01	FLUID, F = 5.0771E-06
1.0000E-01	6.7099E-04	1.0249E-01	-5.4513E-01	FLUID, F = 3.8951E-06
1.7783E-01	1.2547E-03	1.0292E-01	-5.2188E-01	FLUID, F = 3.1758E-06
3.1623E-01	2.4411E-03	1.0380E-01	-4.9699E-01	FLUID, F = 2.8538E-06
5.6234E-01	5.1029E-03	1.0581E-01	-4.6884E-01	FLUID, F = 3.0064E-06
1.0000E+00	1.2138E-02	1.1093E-01	-4.3367E-01	FLUID, F = 4.1253E-06
1.7783E+00	3.5700E-02	1.2624E-01	-3.8136E-01	FLUID, F = 8.7755E-06
3.1623E+00	1.3478E-01	1.7805E-01	-2.8176E-01	FLUID, F = 3.8002E-05
5.6234E+00	5.7438E-01	3.4805E-01	-5.1386E-02	FLUID, F = 5.1375E-04
1.0000E+01	2.2673E+00	8.2235E-01	4.8560E-01	FLUID, F = 4.1409E-02
1.7783E+01	4.4546E+00	1.3494E+00	1.1724E+00	METALLIC SOLID
3.1623E+01	1.7456E+01	2.5742E+00	2.4816E+00	METALLIC SOLID
5.6234E+01	6.0133E+01	5.1922E+00	5.1531E+00	METALLIC SOLID
1.0000E+02	1.9070E+02	1.0096E+01	1.0083E+01	METALLIC SOLID
1.7783E+02	5.7257E+02	1.8605E+01	1.8601E+01	METALLIC SOLID
3.1623E+02	1.6570E+03	3.2684E+01	3.2683E+01	METALLIC SOLID
5.6234E+02	4.6749E+03	5.5270E+01	5.5270E+01	METALLIC SOLID
1.0000E+03	1.2954E+04	9.0743E+01	9.0743E+01	METALLIC SOLID

TEMPERATURE = 3.1623E+03 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	1.1600E-05	2.3885E-01	-1.3909E+00	FLUID, F = 3.5141E-02
1.7783E-03	2.0455E-05	2.2874E-01	-1.3518E+00	FLUID, F = 2.5908E-02
3.1623E-03	3.6156E-05	2.2111E-01	-1.3129E+00	FLUID, F = 1.8943E-02
5.6234E-03	6.4050E-05	2.1540E-01	-1.2743E+00	FLUID, F = 1.3729E-02
1.0000E-02	1.1373E-04	2.1118E-01	-1.2358E+00	FLUID, F = 9.8677E-03
1.7783E-02	2.0253E-04	2.0813E-01	-1.1972E+00	FLUID, F = 7.0519E-03
3.1623E-02	3.6218E-04	2.0601E-01	-1.1586E+00	FLUID, F = 5.0369E-03
5.6234E-02	6.5196E-04	2.0466E-01	-1.1196E+00	FLUID, F = 3.6255E-03
1.0000E-01	1.1866E-03	2.0401E-01	-1.0799E+00	FLUID, F = 2.6596E-03
1.7783E-01	2.2010E-03	2.0412E-01	-1.0390E+00	FLUID, F = 2.0189E-03
3.1623E-01	4.2200E-03	2.0531E-01	-9.9560E-01	FLUID, F = 1.6199E-03
5.6234E-01	8.5772E-03	2.0852E-01	-9.4756E-01	FLUID, F = 1.4202E-03
1.0000E+00	1.9311E-02	2.1644E-01	-8.8995E-01	FLUID, F = 1.4361E-03
1.7783E+00	5.1496E-02	2.3738E-01	-8.1069E-01	FLUID, F = 1.8339E-03
3.1623E+00	1.7059E-01	2.9887E-01	-6.7701E-01	FLUID, F = 3.4519E-03
5.6234E+00	6.4953E-01	4.8345E-01	-4.0436E-01	FLUID, F = 1.2456E-02
1.0000E+01	2.3627E+00	9.7555E-01	1.7449E-01	FLUID, F = 1.2357E-01
1.7783E+01	4.8919E+00	1.5074E+00	9.8588E-01	METALLIC SOLID
3.1623E+01	1.8058E+01	2.7099E+00	2.3690E+00	METALLIC SOLID
5.6234E+01	6.0865E+01	5.2910E+00	5.0950E+00	METALLIC SOLID
1.0000E+02	1.9140E+02	1.0152E+01	1.0059E+01	METALLIC SOLID
1.7783E+02	5.7307E+02	1.8628E+01	1.8593E+01	METALLIC SOLID
3.1623E+02	1.6573E+03	3.2691E+01	3.2680E+01	METALLIC SOLID
5.6234E+02	4.6750E+03	5.5272E+01	5.5269E+01	METALLIC SOLID
1.0000E+03	1.2954E+04	9.0743E+01	9.0742E+01	METALLIC SOLID

TABLE II. CONTINUED.

TEMPERATURE = 5.6234E+03 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	3.4645E-05	1.1521E+00	-2.9104E+00	FLUID, F = 7.1487E-01
1.7783E-03	5.8287E-05	1.0471E+00	-2.7962E+00	FLUID, F = 6.1480E-01
3.1623E-03	9.7416E-05	9.3727E-01	-2.6885E+00	FLUID, F = 5.1029E-01
5.6234E-03	1.6243E-04	8.3132E-01	-2.5875E+00	FLUID, F = 4.0976E-01
1.0000E-02	2.7129E-04	7.3571E-01	-2.4927E+00	FLUID, F = 3.1942E-01
1.7783E-02	4.5550E-04	6.5405E-01	-2.4035E+00	FLUID, F = 2.4273E-01
3.1623E-02	7.7140E-04	5.8755E-01	-2.3189E+00	FLUID, F = 1.8074E-01
5.6234E-02	1.3225E-03	5.3580E-01	-2.2379E+00	FLUID, F = 1.3280E-01
1.0000E-01	2.3057E-03	4.9736E-01	-2.1592E+00	FLUID, F = 9.7219E-02
1.7783E-01	4.1154E-03	4.7043E-01	-2.0811E+00	FLUID, F = 7.1799E-02
3.1623E-01	7.6009E-03	4.5335E-01	-2.0015E+00	FLUID, F = 5.4347E-02
5.6234E-01	1.4792E-02	4.4549E-01	-1.9168E+00	FLUID, F = 4.3047E-02
1.0000E+00	3.1337E-02	4.4879E-01	-1.8204E+00	FLUID, F = 3.6762E-02
1.7783E+00	7.6327E-02	4.7171E-01	-1.6974E+00	FLUID, F = 3.5546E-02
3.1623E+00	2.2496E-01	5.4193E-01	-1.5115E+00	FLUID, F = 4.2589E-02
5.6234E+00	7.6353E-01	7.3403E-01	-1.1747E+00	FLUID, F = 7.4910E-02
1.0000E+01	2.5594E+00	1.2177E+00	-5.2752E-01	FLUID, F = 2.4015E-01
1.7783E+01	5.7233E+00	1.8082E+00	4.8592E-01	METALLIC SOLID
3.1623E+01	1.9324E+01	2.9949E+00	2.0156E+00	METALLIC SOLID
5.6234E+01	6.2742E+01	5.5443E+00	4.8661E+00	METALLIC SOLID
1.0000E+02	1.9391E+02	1.0350E+01	9.9294E+00	METALLIC SOLID
1.7783E+02	5.7582E+02	1.8754E+01	1.8532E+01	METALLIC SOLID
3.1623E+02	1.6595E+03	3.2751E+01	3.2657E+01	METALLIC SOLID
5.6234E+02	4.6765E+03	5.5294E+01	5.5261E+01	METALLIC SOLID
1.0000E+03	1.2955E+04	9.0750E+01	9.0740E+01	METALLIC SOLID

TEMPERATURE = 1.0000E+04 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	7.1294E-05	1.7363E+00	-6.3189E+00	FLUID, F = 9.8922E-01
1.7783E-03	1.2678E-04	1.7260E+00	-6.0774E+00	FLUID, F = 9.8080E-01
3.1623E-03	2.2516E-04	1.7113E+00	-5.8361E+00	FLUID, F = 9.6606E-01
5.6234E-03	3.9852E-04	1.6877E+00	-5.5955E+00	FLUID, F = 9.4084E-01
1.0000E-02	7.0065E-04	1.6490E+00	-5.3567E+00	FLUID, F = 8.9952E-01
1.7783E-02	1.2182E-03	1.5882E+00	-5.1218E+00	FLUID, F = 8.3638E-01
3.1623E-02	2.0860E-03	1.5013E+00	-4.8939E+00	FLUID, F = 7.4908E-01
5.6234E-02	3.5145E-03	1.3918E+00	-4.6762E+00	FLUID, F = 6.4233E-01
1.0000E-01	5.8557E-03	1.2711E+00	-4.4712E+00	FLUID, F = 5.2782E-01
1.7783E-01	9.7644E-03	1.1541E+00	-4.2793E+00	FLUID, F = 4.1927E-01
3.1623E-01	1.6623E-02	1.0536E+00	-4.0979E+00	FLUID, F = 3.2685E-01
5.6234E-01	2.9559E-02	9.7658E-01	-3.9208E+00	FLUID, F = 2.5511E-01
1.0000E+00	5.6708E-02	9.2740E-01	-3.7373E+00	FLUID, F = 2.0418E-01
1.7783E+00	1.2369E-01	9.1279E-01	-3.5269E+00	FLUID, F = 1.7353E-01
3.1623E+00	3.2421E-01	9.5761E-01	-3.2449E+00	FLUID, F = 1.6666E-01
5.6234E+00	9.8165E-01	1.1278E+00	-2.7888E+00	FLUID, F = 2.0676E-01
1.0000E+01	2.9580E+00	1.5917E+00	-2.0066E+00	FLUID, F = 3.7510E-01
1.7783E+01	7.5764E+00	2.4471E+00	-7.8944E-01	FLUID, F = 7.9905E-01
3.1623E+01	2.2179E+01	3.8284E+00	1.0522E+00	FLUID, F = 9.9117E-01
5.6234E+01	6.6563E+01	6.0603E+00	4.1781E+00	METALLIC SOLID
1.0000E+02	1.9988E+02	1.0822E+01	9.4581E+00	METALLIC SOLID
1.7783E+02	5.8442E+02	1.9146E+01	1.8245E+01	METALLIC SOLID
3.1623E+02	1.6701E+03	3.3026E+01	3.2509E+01	METALLIC SOLID
5.6234E+02	4.6865E+03	5.5443E+01	5.5199E+01	METALLIC SOLID
1.0000E+03	1.2962E+04	9.0811E+01	9.0718E+01	METALLIC SOLID

TABLE II. CONTINUED.

TEMPERATURE = 1.7783E+04 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	1.4125E-04	3.1144E+00	-1.2907E+01	FLUID, F = 9.9926E-01
1.7783E-03	2.4552E-04	2.9017E+00	-1.2435E+01	FLUID, F = 9.9850E-01
3.1623E-03	4.2945E-04	2.7385E+00	-1.1971E+01	FLUID, F = 9.9706E-01
5.6234E-03	7.5528E-04	2.6143E+00	-1.1514E+01	FLUID, F = 9.9432E-01
1.0000E-02	1.3343E-03	2.5195E+00	-1.1061E+01	FLUID, F = 9.8919E-01
1.7783E-02	2.3645E-03	2.4450E+00	-1.0610E+01	FLUID, F = 9.7967E-01
3.1623E-02	4.1932E-03	2.3811E+00	-1.0160E+01	FLUID, F = 9.6228E-01
5.6234E-02	7.4118E-03	2.3156E+00	-9.7124E+00	FLUID, F = 9.3150E-01
1.0000E-01	1.2986E-02	2.2347E+00	-9.2690E+00	FLUID, F = 8.8031E-01
1.7783E-01	2.2440E-02	2.1266E+00	-8.8350E+00	FLUID, F = 8.0361E-01
3.1623E-01	3.8371E-02	1.9910E+00	-8.4158E+00	FLUID, F = 7.0402E-01
5.6234E-01	6.5846E-02	1.8431E+00	-8.0129E+00	FLUID, F = 5.9460E-01
1.0000E+00	1.1704E-01	1.7079E+00	-7.6184E+00	FLUID, F = 4.9197E-01
1.7783E+00	2.2859E-01	1.6135E+00	-7.2066E+00	FLUID, F = 4.1155E-01
3.1623E+00	5.2434E-01	1.5995E+00	-6.7210E+00	FLUID, F = 3.6706E-01
5.6234E+00	1.3910E+00	1.7482E+00	-6.0345E+00	FLUID, F = 3.9192E-01
1.0000E+01	3.6798E+00	2.2148E+00	-5.0040E+00	FLUID, F = 5.3270E-01
1.7783E+01	9.1721E+00	3.1196E+00	-3.5241E+00	FLUID, F = 7.9110E-01
3.1623E+01	2.5128E+01	4.6100E+00	-1.3598E+00	FLUID, F = 9.6063E-01
5.6234E+01	7.3571E+01	7.4242E+00	2.1234E+00	FLUID, F = 9.9671E-01
1.0000E+02	2.1478E+02	1.2531E+01	7.8657E+00	FLUID, F = 9.9988E-01
1.7783E+02	6.1580E+02	2.1240E+01	1.7203E+01	FLUID, F = 1.0000E+00
3.1623E+02	1.6992E+03	3.3788E+01	3.1879E+01	METALLIC SOLID
5.6234E+02	4.7255E+03	5.6025E+01	5.4844E+01	METALLIC SOLID
1.0000E+03	1.3004E+04	9.1169E+01	9.0552E+01	METALLIC SOLID

TEMPERATURE = 3.1623E+04 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	3.8439E-04	9.1867E+00	-2.7225E+01	FLUID, F = 9.9999E-01
1.7783E-03	6.4637E-04	8.3759E+00	-2.5958E+01	FLUID, F = 9.9998E-01
3.1623E-03	1.0818E-03	7.5411E+00	-2.4764E+01	FLUID, F = 9.9993E-01
5.6234E-03	1.8105E-03	6.7464E+00	-2.3640E+01	FLUID, F = 9.9978E-01
1.0000E-02	3.0430E-03	6.0355E+00	-2.2581E+01	FLUID, F = 9.9938E-01
1.7783E-02	5.1524E-03	5.4293E+00	-2.1576E+01	FLUID, F = 9.9840E-01
3.1623E-02	9.8046E-03	4.9304E+00	-2.0615E+01	FLUID, F = 9.9615E-01
5.6234E-02	1.5189E-02	4.5286E+00	-1.9687E+01	FLUID, F = 9.9123E-01
1.0000E-01	2.6418E-02	4.2056E+00	-1.8783E+01	FLUID, F = 9.8092E-01
1.7783E-01	4.6169E-02	3.9360E+00	-1.7896E+01	FLUID, F = 9.6038E-01
3.1623E-01	8.0751E-02	3.6904E+00	-1.7024E+01	FLUID, F = 9.2250E-01
5.6234E-01	1.4098E-01	3.4437E+00	-1.6167E+01	FLUID, F = 8.6104E-01
1.0000E+00	2.4756E-01	3.1902E+00	-1.5325E+01	FLUID, F = 7.7662E-01
1.7783E+00	4.5319E-01	2.9623E+00	-1.4478E+01	FLUID, F = 6.8468E-01
3.1623E+00	9.2055E-01	2.8306E+00	-1.3569E+01	FLUID, F = 6.1302E-01
5.6234E+00	2.1226E+00	2.9271E+00	-1.2451E+01	FLUID, F = 6.1287E-01
1.0000E+01	4.9527E+00	3.3854E+00	-1.0983E+01	FLUID, F = 7.0793E-01
1.7783E+01	1.1604E+01	4.2954E+00	-9.0624E+00	FLUID, F = 8.4821E-01
3.1623E+01	2.9820E+01	5.8757E+00	-6.4106E+00	FLUID, F = 9.4530E-01
5.6234E+01	8.1721E+01	8.7586E+00	-2.4288E+00	FLUID, F = 9.8710E-01
1.0000E+02	2.2884E+02	1.3903E+01	3.7961E+00	FLUID, F = 9.9854E-01
1.7783E+02	6.4052E+02	2.2657E+01	1.3606E+01	FLUID, F = 1.0000E+00
3.1623E+02	1.7789E+03	3.6991E+01	2.8987E+01	FLUID, F = 1.0000E+00
5.6234E+02	4.8951E+03	5.9842E+01	5.2889E+01	FLUID, F = 1.0000E+00
1.0000E+03	1.3354E+04	9.5591E+01	8.9702E+01	FLUID, F = 1.0000E+00

TABLE II. CONTINUED.

TEMPERATURE = 5.6234E+04 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	7.8584E-04	1.4429E+01	-5.7579E+01	FLUID, F = 1.0000E+00
1.7783E-03	1.3856E-03	1.4253E+01	-5.4928E+01	FLUID, F = 1.0000E+00
3.1623E-03	2.4299E-03	1.3968E+01	-5.2307E+01	FLUID, F = 1.0000E+00
5.6234E-03	4.2281E-03	1.3532E+01	-4.9731E+01	FLUID, F = 1.0000E+00
1.0000E-02	7.2859E-03	1.2917E+01	-4.7223E+01	FLUID, F = 9.9999E-01
1.7783E-02	1.2428E-02	1.2128E+01	-4.4804E+01	FLUID, F = 9.9998E-01
3.1623E-02	2.1024E-02	1.1213E+01	-4.2495E+01	FLUID, F = 9.9990E-01
5.6234E-02	3.5416E-02	1.0251E+01	-4.0303E+01	FLUID, F = 9.9965E-01
1.0000E-01	5.9718E-02	9.3194E+00	-3.8227E+01	FLUID, F = 9.9885E-01
1.7783E-01	1.0127E-01	8.4757E+00	-3.6253E+01	FLUID, F = 9.9656E-01
3.1623E-01	1.7326E-01	7.7425E+00	-3.4363E+01	FLUID, F = 9.9065E-01
5.6234E-01	2.9937E-01	7.1127E+00	-3.2536E+01	FLUID, F = 9.7704E-01
1.0000E+00	5.2266E-01	6.5589E+00	-3.0751E+01	FLUID, F = 9.4939E-01
1.7783E+00	9.2959E-01	6.0656E+00	-2.8985E+01	FLUID, F = 9.0380E-01
3.1623E+00	1.7340E+00	5.6794E+00	-2.7185E+01	FLUID, F = 8.5001E-01
5.6234E+00	3.5124E+00	5.5774E+00	-2.5214E+01	FLUID, F = 8.3153E-01
1.0000E+01	7.3655E+00	5.8850E+00	-2.2920E+01	FLUID, F = 8.6899E-01
1.7783E+01	1.6004E+01	6.6469E+00	-2.0174E+01	FLUID, F = 9.2252E-01
3.1623E+01	3.7748E+01	8.1482E+00	-1.6677E+01	FLUID, F = 9.6046E-01
5.6234E+01	9.5595E+01	1.1026E+01	-1.1852E+01	FLUID, F = 9.8404E-01
1.0000E+02	2.5292E+02	1.6202E+01	-4.8015E+00	FLUID, F = 9.9660E-01
1.7783E+02	6.8243E+02	2.5001E+01	5.8142E+00	FLUID, F = 1.0000E+00
3.1623E+02	1.8531E+03	3.9390E+01	2.1990E+01	FLUID, F = 1.0000E+00
5.6234E+02	5.0272E+03	6.2307E+01	4.6686E+01	FLUID, F = 1.0000E+00
1.0000E+03	1.3591E+04	9.8137E+01	8.4298E+01	FLUID, F = 1.0000E+00

TEMPERATURE = 1.0000E+05 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	1.4121E-03	2.0098E+01	-1.1545E+02	FLUID, F = 1.0000E+00
1.7783E-03	2.5089E-03	2.0070E+01	-1.1067E+02	FLUID, F = 1.0000E+00
3.1623E-03	4.4540E-03	2.0019E+01	-1.0589E+02	FLUID, F = 1.0000E+00
5.6234E-03	7.8963E-03	1.9931E+01	-1.0113E+02	FLUID, F = 1.0000E+00
1.0000E-02	1.3966E-02	1.9777E+01	-9.6386E+01	FLUID, F = 1.0000E+00
1.7783E-02	2.4608E-02	1.9521E+01	-9.1676E+01	FLUID, F = 1.0000E+00
3.1623E-02	4.3109E-02	1.9112E+01	-8.7023E+01	FLUID, F = 1.0000E+00
5.6234E-02	7.4935E-02	1.8502E+01	-8.2456E+01	FLUID, F = 9.9999E-01
1.0000E-01	1.2911E-01	1.7670E+01	-7.8011E+01	FLUID, F = 9.9997E-01
1.7783E-01	2.2068E-01	1.6645E+01	-7.3722E+01	FLUID, F = 9.9988E-01
3.1623E-01	3.7555E-01	1.5507E+01	-6.9610E+01	FLUID, F = 9.9951E-01
5.6234E-01	6.3978E-01	1.4359E+01	-6.5675E+01	FLUID, F = 9.9829E-01
1.0000E+00	1.0976E+00	1.3287E+01	-6.1894E+01	FLUID, F = 9.9476E-01
1.7783E+00	1.9086E+00	1.2344E+01	-5.8224E+01	FLUID, F = 9.8634E-01
3.1623E+00	3.3984E+00	1.1573E+01	-5.4598E+01	FLUID, F = 9.7145E-01
5.6234E+00	6.3090E+00	1.1103E+01	-5.0894E+01	FLUID, F = 9.6055E-01
1.0000E+01	1.2202E+01	1.1069E+01	-4.6944E+01	FLUID, F = 9.6499E-01
1.7783E+01	2.4659E+01	1.1541E+01	-4.2556E+01	FLUID, F = 9.7504E-01
3.1623E+01	5.2970E+01	1.2778E+01	-3.7416E+01	FLUID, F = 9.8305E-01
5.6234E+01	1.2152E+02	1.5374E+01	-3.0991E+01	FLUID, F = 9.9022E-01
1.0000E+02	2.9627E+02	2.0313E+01	-2.2427E+01	FLUID, F = 9.9695E-01
1.7783E+02	7.5565E+02	2.9002E+01	-1.0383E+01	FLUID, F = 1.0000E+00
3.1623E+02	1.9806E+03	4.3404E+01	7.1701E+00	FLUID, F = 1.0000E+00
5.6234E+02	5.2526E+03	6.6388E+01	3.3227E+01	FLUID, F = 1.0000E+00
1.0000E+03	1.3992E+04	1.0230E+02	7.2195E+01	FLUID, F = 1.0000E+00

TABLE II. CONTINUED.

TEMPERATURE = 1.7783E+05 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	2.5137E-03	2.9833E+01	-2.2401E+02	FLUID, F = 1.0000E+00
1.7783E-03	4.4697E-03	2.9828E+01	-2.1550E+02	FLUID, F = 1.0000E+00
3.1623E-03	7.9470E-03	2.9817E+01	-2.0699E+02	FLUID, F = 1.0000E+00
5.6234E-03	1.4126E-02	2.9796E+01	-1.9848E+02	FLUID, F = 1.0000E+00
1.0000E-02	2.5101E-02	2.9756E+01	-1.8998E+02	FLUID, F = 1.0000E+00
1.7783E-02	4.4566E-02	2.9684E+01	-1.8148E+02	FLUID, F = 1.0000E-00
3.1623E-02	7.9016E-02	2.9554E+01	-1.7301E+02	FLUID, F = 1.0000E+00
5.6234E-02	1.3976E-01	2.9329E+01	-1.6457E+02	FLUID, F = 1.0000E+00
1.0000E-01	2.4628E-01	2.8952E+01	-1.5619E+02	FLUID, F = 1.0000E+00
1.7783E-01	4.3156E-01	2.8358E+01	-1.4790E+02	FLUID, F = 1.0000E+00
3.1623E-01	7.5098E-01	2.7493E+01	-1.3977E+02	FLUID, F = 9.9998E-01
5.6234E-01	1.2978E+00	2.6353E+01	-1.3184E+02	FLUID, F = 9.9992E-01
1.0000E+00	2.2332E+00	2.5010E+01	-1.2415E+02	FLUID, F = 9.9967E-01
1.7783E+00	3.8473E+00	2.3598E+01	-1.1671E+02	FLUID, F = 9.9887E-01
3.1623E+00	6.6894E+00	2.2283E+01	-1.0947E+02	FLUID, F = 9.9691E-01
5.6234E+00	1.1865E+01	2.1244E+01	-1.0233E+02	FLUID, F = 9.9463E-01
1.0000E+01	2.1680E+01	2.0674E+01	-9.5111E+01	FLUID, F = 9.9421E-01
1.7783E+01	4.1172E+01	2.0751E+01	-8.7551E+01	FLUID, F = 9.9492E-01
3.1623E+01	8.2026E+01	2.1728E+01	-7.9284E+01	FLUID, F = 9.9561E-01
5.6234E+01	1.7228E+02	2.4046E+01	-6.9770E+01	FLUID, F = 9.9663E-01
1.0000E+02	3.8234E+02	2.8512E+01	-5.8211E+01	FLUID, F = 9.9858E-01
1.7783E+02	8.9657E+02	3.6571E+01	-4.3365E+01	FLUID, F = 1.0000E+00
3.1623E+02	2.2114E+03	5.0476E+01	-2.3241E+01	FLUID, F = 1.0000E+00
5.6234E+02	5.6458E+03	7.3294E+01	5.2267E+00	FLUID, F = 1.0000E+00
1.0000E+03	1.4684E+04	1.0925E+02	4.6546E+01	FLUID, F = 1.0000E+00

TEMPERATURE = 3.1623E+05 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	4.4704E-03	4.7101E+01	-4.2701E+02	FLUID, F = 1.0000E+00
1.7783E-03	7.9499E-03	4.7101E+01	-4.1188E+02	FLUID, F = 1.0000E+00
3.1623E-03	1.4138E-02	4.7100E+01	-3.9674E+02	FLUID, F = 1.0000E+00
5.6234E-03	2.5142E-02	4.7096E+01	-3.8160E+02	FLUID, F = 1.0000E+00
1.0000E-02	4.4708E-02	4.7087E+01	-3.6646E+02	FLUID, F = 1.0000E+00
1.7783E-02	7.9492E-02	4.7067E+01	-3.5132E+02	FLUID, F = 1.0000E+00
3.1623E-02	1.4130E-01	4.7026E+01	-3.3619E+02	FLUID, F = 1.0000E+00
5.6234E-02	2.5104E-01	4.6948E+01	-3.2106E+02	FLUID, F = 1.0000E+00
1.0000E-01	4.4555E-01	4.6800E+01	-3.0596E+02	FLUID, F = 1.0000E+00
1.7783E-01	7.8934E-01	4.6536E+01	-2.9090E+02	FLUID, F = 1.0000E+00
3.1623E-01	1.3943E+00	4.6084E+01	-2.7591E+02	FLUID, F = 1.0000E+00
5.6234E-01	2.4521E+00	4.5356E+01	-2.6106E+02	FLUID, F = 1.0000E+00
1.0000E+00	4.2890E+00	4.4280E+01	-2.4641E+02	FLUID, F = 9.9998E-01
1.7783E+00	7.4636E+00	4.2851E+01	-2.3204E+02	FLUID, F = 9.9993E-01
3.1623E+00	1.2961E+01	4.1182E+01	-2.1799E+02	FLUID, F = 9.9975E-01
5.6234E+00	2.2606E+01	3.9509E+01	-2.0426E+02	FLUID, F = 9.9947E-01
1.0000E+01	3.9964E+01	3.8153E+01	-1.9071E+02	FLUID, F = 9.9930E-01
1.7783E+01	7.2368E+01	3.7473E+01	-1.7708E+02	FLUID, F = 9.9926E-01
3.1623E+01	1.3573E+02	3.7877E+01	-1.6298E+02	FLUID, F = 9.9922E-01
5.6234E+01	2.6600E+02	3.9865E+01	-1.4777E+02	FLUID, F = 9.9926E-01
1.0000E+02	5.4693E+02	4.4101E+01	-1.3060E+02	FLUID, F = 9.9961E-01
1.7783E+02	1.1803E+03	5.1643E+01	-1.1025E+02	FLUID, F = 1.0000E+00
3.1623E+02	2.6788E+03	6.4479E+01	-8.4910E+01	FLUID, F = 1.0000E+00
5.6234E+02	6.3953E+03	8.6053E+01	-5.1687E+01	FLUID, F = 1.0000E+00
1.0000E+03	1.5919E+04	1.2128E+02	-6.0401E+00	FLUID, F = 1.0000E+00

TABLE II. CONTINUED.

TEMPERATURE = 5.6234E+05 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	7.9493E-03	7.7798E+01	-8.0569E+02	FLUID, F = 1.0000E+00
1.7783E-03	1.4137E-02	7.7800E+01	-7.7877E+02	FLUID, F = 1.0000E+00
3.1623E-03	2.5141E-02	7.7803E+01	-7.5185E+02	FLUID, F = 1.0000E+00
5.6234E-03	4.4711E-02	7.7805E+01	-7.2493E+02	FLUID, F = 1.0000E+00
1.0000E-02	7.9516E-02	7.7807E+01	-6.9800E+02	FLUID, F = 1.0000E+00
1.7783E-02	1.4142E-01	7.7807E+01	-6.7108E+02	FLUID, F = 1.0000E+00
3.1623E-02	2.5151E-01	7.7801E+01	-6.4415E+02	FLUID, F = 1.0000E+00
5.6234E-02	4.4728E-01	7.7781E+01	-6.1721E+02	FLUID, F = 1.0000E+00
1.0000E-01	7.9529E-01	7.7734E+01	-5.9028E+02	FLUID, F = 1.0000E+00
1.7783E-01	1.4135E+00	7.7635E+01	-5.6336E+02	FLUID, F = 1.0000E+00
3.1623E-01	2.5102E+00	7.7439E+01	-5.3646E+02	FLUID, F = 1.0000E+00
5.6234E-01	4.4509E+00	7.7073E+01	-5.0961E+02	FLUID, F = 1.0000E+00
1.0000E+00	7.8719E+00	7.6437E+01	-4.8288E+02	FLUID, F = 1.0000E+00
1.7783E+00	1.3871E+01	7.5410E+01	-4.5633E+02	FLUID, F = 1.0000E+00
3.1623E+00	2.4338E+01	7.3915E+01	-4.3009E+02	FLUID, F = 9.9998E-01
5.6234E+00	4.2569E+01	7.2004E+01	-4.0424E+02	FLUID, F = 9.9996E-01
1.0000E+01	7.4535E+01	6.9937E+01	-3.7881E+02	FLUID, F = 9.9993E-01
1.7783E+01	1.3161E+02	6.8188E+01	-3.5369E+02	FLUID, F = 9.9991E-01
3.1623E+01	2.3675E+02	6.7389E+01	-3.2853E+02	FLUID, F = 9.9989E-01
5.6234E+01	4.3870E+02	6.8305E+01	-3.0273E+02	FLUID, F = 9.9988E-01
1.0000E+02	8.4564E+02	7.1845E+01	-2.7532E+02	FLUID, F = 9.9993E-01
1.7783E+02	1.7048E+03	7.9097E+01	-2.4493E+02	FLUID, F = 1.0000E+00
3.1623E+02	3.5966E+03	9.1542E+01	-2.0966E+02	FLUID, F = 1.0000E+00
5.6234E+02	7.9421E+03	1.1178E+02	-1.6682E+02	FLUID, F = 1.0000E+00
1.0000E+03	1.8401E+04	1.4469E+02	-1.1230E+02	FLUID, F = 1.0000E+00

TEMPERATURE = 1.0000E+06 DEGREES KELVIN

COMPRESSION	P MBAR	E MB-CC/GM	A MB-CC/GM	PHASE
1.0000E-03	1.4136E-02	1.3238E+02	-1.5105E+03	FLUID, F = 1.0000E+00
1.7783E-03	2.5138E-02	1.3239E+02	-1.4626E+03	FLUID, F = 1.0000E+00
3.1623E-03	4.4704E-02	1.3239E+02	-1.4148E+03	FLUID, F = 1.0000E+00
5.6234E-03	7.9502E-02	1.3240E+02	-1.3669E+03	FLUID, F = 1.0000E+00
1.0000E-02	1.4139E-01	1.3240E+02	-1.3190E+03	FLUID, F = 1.0000E+00
1.7783E-02	2.5147E-01	1.3241E+02	-1.2711E+03	FLUID, F = 1.0000E+00
3.1623E-02	4.4726E-01	1.3242E+02	-1.2232E+03	FLUID, F = 1.0000E+00
5.6234E-02	7.9553E-01	1.3243E+02	-1.1753E+03	FLUID, F = 1.0000E+00
1.0000E-01	1.4150E+00	1.3244E+02	-1.1274E+03	FLUID, F = 1.0000E+00
1.7783E-01	2.5170E+00	1.3243E+02	-1.0795E+03	FLUID, F = 1.0000E+00
3.1623E-01	4.4765E+00	1.3238E+02	-1.0316E+03	FLUID, F = 1.0000E+00
5.6234E-01	7.9588E+00	1.3225E+02	-9.8366E+02	FLUID, F = 1.0000E+00
1.0000E+00	1.4140E+01	1.3197E+02	-9.3575E+02	FLUID, F = 1.0000E+00
1.7783E+00	2.5084E+01	1.3141E+02	-8.8792E+02	FLUID, F = 1.0000E+00
3.1623E+00	4.4395E+01	1.3044E+02	-8.4026E+02	FLUID, F = 1.0000E+00
5.6234E+00	7.8321E+01	1.2889E+02	-7.9289E+02	FLUID, F = 1.0000E+00
1.0000E+01	1.3774E+02	1.2672E+02	-7.4598E+02	FLUID, F = 9.9999E-01
1.7783E+01	2.4203E+02	1.2418E+02	-6.9963E+02	FLUID, F = 9.9999E-01
3.1623E+01	4.2726E+02	1.2189E+02	-6.5374E+02	FLUID, F = 9.9999E-01
5.6234E+01	7.6438E+02	1.2086E+02	-6.0792E+02	FLUID, F = 9.9998E-01
1.0000E+02	1.4007E+03	1.2238E+02	-5.6131E+02	FLUID, F = 9.9999E-01
1.7783E+02	2.6571E+03	1.2804E+02	-5.1248E+02	FLUID, F = 1.0000E+00
3.1623E+02	5.2567E+03	1.3970E+02	-4.5928E+02	FLUID, F = 1.0000E+00
5.6234E+02	1.0866E+04	1.5965E+02	-3.9875E+02	FLUID, F = 1.0000E+00
1.0000E+03	2.3449E+04	1.9132E+02	-3.2682E+02	FLUID, F = 1.0000E+00

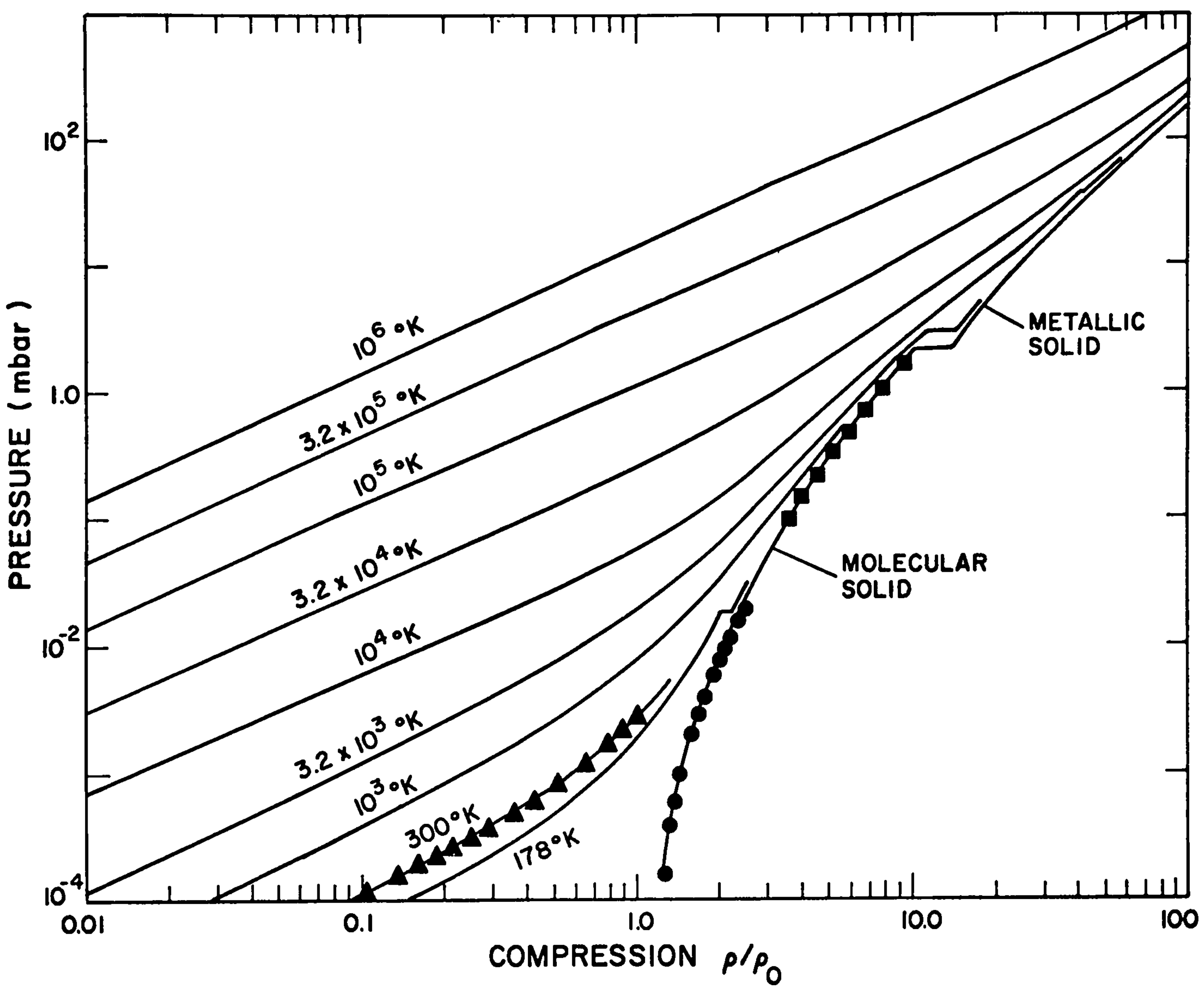

Fig. 10. Pressure isotherms for deuterium. Circles are from Ref. 5, squares from Ref. 6, and triangles from Ref. 27.

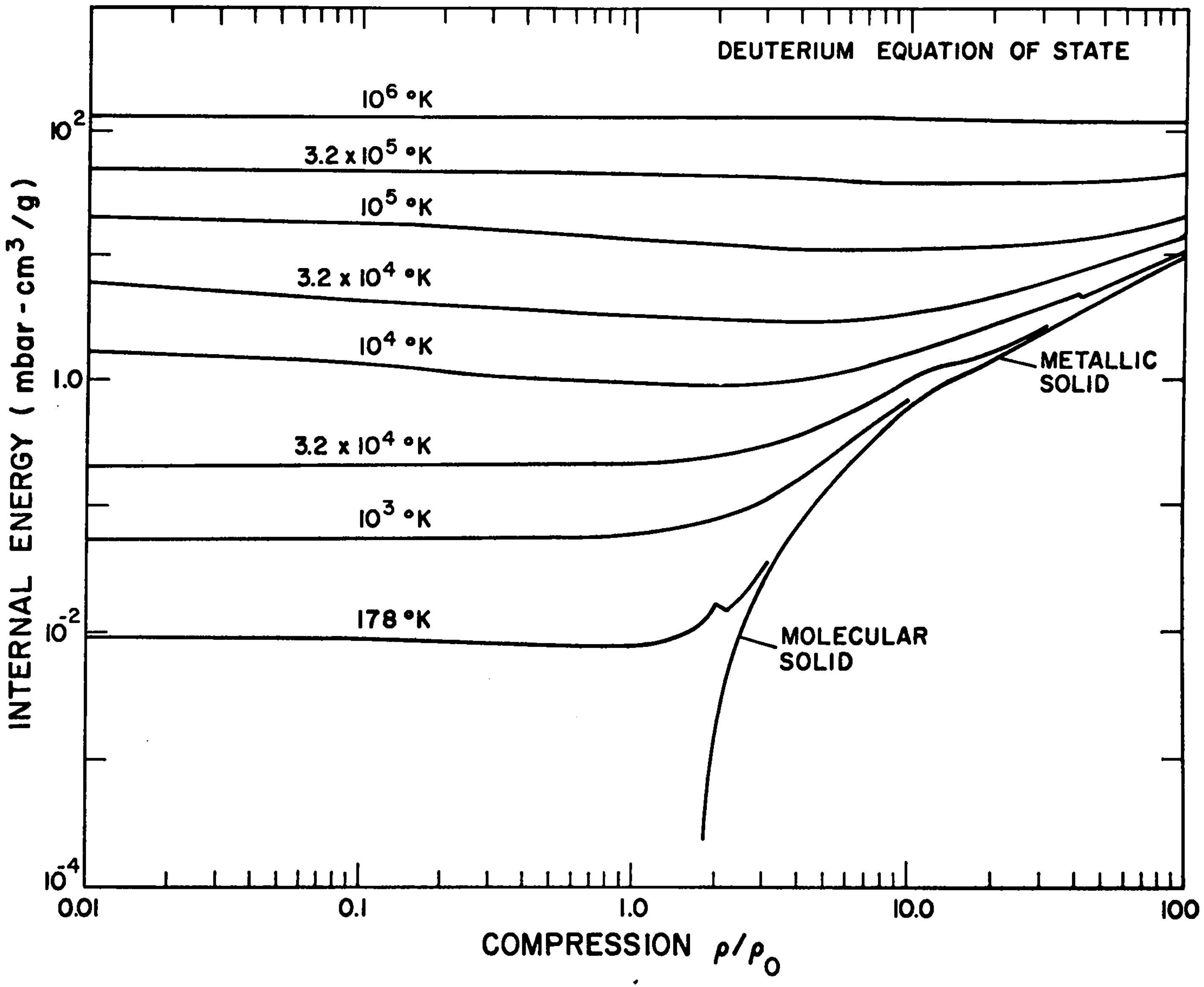

Fig. 11. Internal energy on isotherms for deuterium.

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APPENDIX

PROPERTIES OF A UNIFORM ELECTRON GAS

In this appendix, we summarize a few of the results for an electron gas obeying Fermi-Dirac statistics. A more complete discussion of this problem can be found in standard references.[28]

According to Fermi-Dirac statistics, the number of electrons in a volume V, having energies in the range $\epsilon \rightarrow \epsilon + d\epsilon$, is given by

$$dn = \frac{4\pi V}{h^3} (2m)^{3/2} \frac{\epsilon^{1/2} d\epsilon}{e^{\alpha+\beta\epsilon}+1} , \qquad \text{(A-1)}$$

where $\beta = 1/kT$ and m is the electron mass. The parameter α is determined from the normalization condition, $N = \int dn$. Hence

$$N = 2V \left(\frac{2\pi mkT}{h^2}\right) V(\alpha, 1/2) ,$$

$$V(\alpha,1/2) = \frac{2}{\pi} \int_0^\infty \frac{z^{1/2} dz}{e^{\alpha+Z}+1} . \qquad \text{(A-2)}$$

The energy and pressure are given by

$$E = \int \epsilon \, dn = \frac{3}{2} NkT \frac{V(\alpha,3/2)}{V(\alpha, 1/2)} ,$$

$$P = \frac{2}{3} \frac{E}{V} ,$$

$$V(\alpha,3/2) = \frac{4}{3\sqrt{\pi}} \int_0^\infty \frac{z^{3/2} dz}{e^{\alpha+Z}+1} . \qquad \text{(A-3)}$$

The Helmholtz free energy can be shown to be

$$A = -NkT \ln q$$

$$= \frac{4\pi V}{Nh^3} (2m)^{3/2} \int_0^\infty \epsilon^{1/2} \ln \left(1+e^{-\alpha-\beta\epsilon}\right) d\epsilon + \alpha , \qquad \text{(A-4)}$$

where q is defined to be the electron partition function. To verify Eq. (A-4), we note that it satisfies the thermodynamic relation,

$$E = - T^2 \frac{\partial}{\partial T}\left(\frac{A}{T}\right)_V , \qquad \text{(A-5)}$$

and also that the entropy $S = (E-A)/T$ vanishes as $T \rightarrow 0$.

In order to eliminate the parameter α from the above equations, we introduce the function

$$y(V,T) = \frac{h^2}{2\pi mkT} \left(\frac{N}{2V}\right)^{2/3} . \qquad \text{(A-6)}$$

From Eq. (A-2), it follows that

$$V(\alpha,1/2) = y(V,T)^{3/2} . \qquad \text{(A-7)}$$

It can be shown that, at high temperatures and/or low densities,[28]

$$\frac{V(\alpha,3/2)}{V(\alpha,1/2)} \rightarrow 1 - .1768\, y - .0038\, y^2 \ldots .$$

At low temperatures and/or high densities, we have the following asymptotic expression.

$$\frac{V(\alpha,3/2)}{V(\alpha,1/2)} \rightarrow \frac{h^2}{5mkT} \left(\frac{3N}{8\pi V}\right)^{2/3} + 1.3606y \ldots .$$

Let us write the energy in the form

$$E(V,T) = E_F(V) + \frac{3}{2} NkT\, F(y) ,$$

$$E_F(V) = \frac{3Nh^2}{10m} \left(\frac{3N}{8\pi V}\right)^{2/3} = \frac{3}{2} NkT\, (.4836y) ,$$

$$F(y) = \frac{V(\alpha,3/2)}{V(\alpha,1/2)} - .4836y . \qquad \text{(A-8)}$$

$E_F(V)$ is the Fermi energy, or zero-point energy of the electrons. The term involving F(y) gives the temperature-dependent contribution to the equation of state.

We next calculate the functions F(y) and y for a number of values of α. F(y) is shown as a function of y in Fig. A1. We find that this function can be fit remarkably well by the formula

$$F(y) = \frac{1 + (b/2)y}{1 + by + cy^2} \; , \qquad \text{(A-9)}$$

where b = 2.7212 c. The value of c will be determined shortly. The Helmholtz free energy can be derived by integrating Eq. (A-5). The result is

$$A = - NkT \ln q_e + E_F(V) \quad , \qquad \text{(A-10)}$$

where

$$q_e = \left[\frac{1 + by + cy^2}{cy^2}\right]^{3/4} \quad . \qquad \text{(A-11)}$$

To determine the constant c, we require that q_e approach the classical limit, Eq. (54), as $T \to \infty$ and $y \to o$.

$$q_e \to \frac{1}{C^{3/4} y^{3/2}} = \frac{1}{C^{3/4} e} \frac{2eV}{N} \left(\frac{2\pi mkT}{h^2}\right)^{3/2} ,$$

as $y \to o$. Hence, $c = e^{-4/3} = .2636$.

Our approximate expression for F(y) is compared with the exact function in Fig. A1. Equations (A-9) and (A-11), for F(y) and $q_e(y)$, fit the exact expressions with a maximum error of 3%.

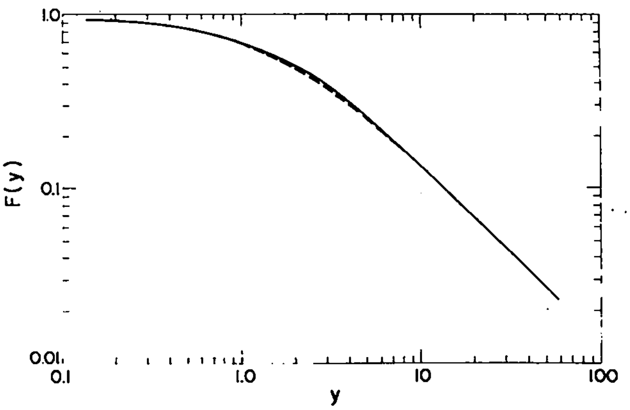

Fig. A1. The function F(y). The solid curve is the exact result. The dashed line is our analytic expression, Eq. (A-9).

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