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THERMODYNAMIC PROPERTIES OF HYDROGEN FROM ROOM TEMPERATURE TO 100,000° K

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SUMMARY

Expressions for the composition, specific volume, enthalpy, and entropy of hydrogen gas have been derived, and equilibrium values of these quantities have been tabulated for temperatures ranging from room temperature (300° K) to 100,000° K and for pressures from 10^{-5} to 10^{2} atmospheres. A new method of calculating the internal partition function of diatomic hydrogen by using a Morse potential to approximate the forces between the two nuclei results in a series that converges much more rapidly at a given temperature than the summing over the vibration-rotation energy levels usually employed.

INTRODUCTION

The determination of the thrust obtained in high-temperature rockets requires a knowledge of the thermodynamic properties of the working fluid at the temperatures involved. These temperatures might conceivably range up to, or even above, 100,000° K.

Because of the simplicity of the structure of the hydrogen atom and molecule, the properties of hydrogen may be calculated fairly accurately in the very high temperature region where no experimental data are available. The National Bureau of Standards (ref. 1) has tabulated values up to 5000° K; Sänger-Bredt (ref. 2) presents charts for temperatures up to 10,000° K; and Altman (ref. 3) has completed calculations up to 20,000° K. However, tabulated values such as those given in reference 1 are not available for temperatures above 5000° K. Table I of this report offers such values for temperatures ranging from room temperature to 100,000° K and for pressures from 10^{-5} to 10^{2} atmospheres. The properties listed include composition, specific volume, enthalpy, and entropy. Sufficient entries have been made to allow interpolation for temperatures and pressures not explicitly tabulated.

The calculation of the internal partition function of the diatomic hydrogen molecule normally involves a summing over a large number of the vibration-rotation energy levels that characterize the interaction between the two nuclei. The number of levels that must be considered increases rapidly with the temperature, and the convergence of the sum above 4000° K is extremely slow. A new method of treating this problem is given in appendix A, wherein the forces between the nuclei are approximated by a Morse potential. The application of old quantum-theory methods results in a series for the internal partition function that converges much more rapidly than the aforementioned summation.

ANALYSIS

In determining the equilibrium properties of hydrogen at high temperature, two almost independent processes must be considered: (1) dissociation of the hydrogen molecule into its two atomic components, and (2) electronic excitation and ionization of the free atoms. From room temperature to about 1500° K, hydrogen is a diatomic gas where the molecule is essentially in its lowest vibrational state. Above 1500° K, the excited vibrational states start to fill up, and the vibrational amplitude and average distance of separation of the two nuclei in the molecule increase rapidly with temperature. In addition, the probability of finding a free or nascent hydrogen atom also increases until, at 10,000° K, the dissociation process is complete and the gas, in the main, exists as uncoupled hydrogen atoms. Above 10,000° K, the second process comes into play; and, at 90,000° K and a pressure of 100 atmospheres, the gas is 99 percent ionized and can be treated as a plasma of free electrons and protons.

It should be noted that throughout this report the amount of any singly ionized diatomic hydrogen or molecular hydrogen with excited electronic states is considered as negligible because the energy needed to excite the electrons is larger than that necessary for dissociation.

Consider the system as composed of a total of M hydrogen nuclei and M electrons at a given volume V and temperature T. The dissociation process is represented by the reaction

$$H_2 \rightarrow 2H \tag{1}$$

and the ionization process by

$$H \rightarrow p^+ + e^- \tag{2}$$

Let α be the fraction of hydrogen nuclei (or electrons) that are present as hydrogen molecules, so that $N_2 = \frac{\alpha M}{2}$ is the number of

hydrogen molecules. Let β be the fraction of hydrogen nuclei that are free, that is, exist as protons. Then $N_p = \beta M$ is the number of protons. The number of free electrons is also given by $N_e = \beta M$. The remaining nuclei and electrons are present as hydrogen atoms, which number $N_H = (1 - \beta - \alpha)M$. The total number of separate particles in the system is equal to

$$N = \left(1 + \beta - \frac{\alpha}{2}\right)M$$

If the gas is ideal in the sense that no interaction between the particles of the gas need be considered, the partition function of the system can be written as

$$Z = \frac{(z_2)^{N_2}}{N_2!} \frac{(z_H)^{N_H}}{N_H!} \frac{(z_p)^{N_p}}{N_p!} \frac{(z_e)^{N_e}}{N_e!} \tag{3}$$

where z_2, z_H, z_p, and z_e are the respective partition functions for an individual hydrogen molecule, a hydrogen atom, a proton, and an electron.

If the multiplicity associated with the nuclear spins is neglected and it is assumed that only normal hydrogen is involved, that is, the ortho- to parahydrogen ratio is 3 to 1, the partition function z_2 may be written as

$$z_2 = \frac{V}{h^3} (2\pi m_2 kT)^{3/2} z_{vr} \tag{4}$$

where k is the Boltzmann gas constant, h is Planck's constant, m_2 is the mass of a hydrogen molecule, and z_{vr}, the internal partition function for the molecule, is the contribution of the vibrational and rotational degrees of freedom. Here the zero level of energy is taken as that of the hydrogen molecule in its ground state.

Under the same assumptions, the partition function z_H is

$$z_H = \frac{V}{h^3} (2\pi m_H kT)^{3/2} e^{-q/2kT} z_o \tag{5}$$

where m_H is the mass of a hydrogen atom, q is the energy of dissociation of a hydrogen molecule at 0° K, and z_o, the internal partition function, is the contribution of the orbital electronic motion.

The partition function z_p is given by

$$z_p = \frac{V}{h^3} (2\pi m_p kT)^{3/2} e^{-q/2kT} \tag{6}$$

where m_p is the mass of a proton, and the partition function z_e is given by

$$z_e = \frac{2V}{h^3} (2\pi m_e kT)^{3/2} e^{-I/kT} \tag{7}$$

where m_e is the electronic mass and I is the energy needed to ionize a hydrogen atom in its ground state. Note that in equations (6) and (7) it is assumed for convenience that the electron possesses all the ionization energy and the proton all the dissociation energy.

The internal partition function z_{vr} for the hydrogen molecule is considered in appendix A and may be approximated by the following expression (see appendix A):

$$\begin{aligned} z_{vr} = {} & 0.25 + 5.436\times10^{-3}\, T \sum_v e^{-E_v/kT} \\ & + 14.1\times10^{-3} T\, e^{3.202\times10^3/T} \sum_{n=2}^{\infty} (2r_o a A_{2n} + B_{2n})(0.018118\times10^{-3}\, T)^n\, I_n\left(\frac{6.313\times10^3}{T}, \frac{55.194\times10^3}{T}\right) \\ & + 0.8306\times10^{-3} T\, e^{3.202\times10^3/T} \sum_{n=1}^{\infty} (2r_o a C_{2n} + D_{2n})(0.018118\times10^{-3}\, T)^n\, I_n\left(\frac{3.202\times10^3}{T}, \frac{6.313\times10^3}{T}\right) \end{aligned} \tag{8}$$

where E_v is the energy of the lowest lying level corresponding to a vibrational quantum number of v (table II), $(2r_o a A_{2n} + B_{2n})$ and $(2r_o a C_{2n} + D_{2n})$ are constants (tables III and IV), and

$$I_n(x,y) \equiv \int_x^y \zeta^n e^{-\zeta}\, d\zeta$$

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The internal partition function z_o of the hydrogen atom is a function of both pressure and temperature and may be approximated by (see appendix B):

$$z_o = e^{-C/T}\left[2e^{C/T} + 8e^{C/4T} - 10.08 - \frac{5C}{T} + \frac{0.3939}{\sqrt{b}} + \left(1.613\,\frac{C}{T} - 0.7652\right)\frac{1}{b^{1/6}} - 1.174\,\frac{C}{T}\,b^{1/6}\right] \tag{9}$$

where

$$C = 15.77\times10^{4}\ {}^{\circ}K$$

$$b = 4.555\times10^{-3}\,\frac{P_{atm}}{T}$$

and where P_{atm} is the pressure in atmospheres.

The partition function for the system as given by equation (3) can be written in terms of α and β. Actually, it is more convenient to employ the natural logarithm of the partition function:

$$\ln Z = \frac{\alpha M}{2}\ln\frac{z_2}{\frac{\alpha}{2}M} + M(1-\alpha-\beta)\ln\frac{z_H}{(1-\beta-\alpha)M} + \beta M\ln\frac{z_e z_p}{(\beta M)^2} + \left(1+\beta-\frac{\alpha}{2}\right)M \tag{10}$$

where Stirling's approximation to the factorial has been used.

The equation of equilibrium with respect to reaction (1) is obtained by setting the partial derivative of $\ln Z$ with respect to α equal to zero:

$$\frac{z_2}{\frac{\alpha}{2}M} = \left[\frac{z_H}{(1-\beta-\alpha)M}\right]^2 \exp\left[-2(1-\alpha-\beta)\left(\frac{\partial \ln z_o}{\partial\alpha}\right)_{T,V,\beta}\right] \tag{11}$$

Similarly, the equation of equilibrium with respect to reaction (2) is obtained by setting the partial derivative of $\ln Z$ with respect to β equal to zero:

$$\frac{z_e z_p}{(\beta M)^2} = \frac{z_H}{(1-\beta-\alpha)M}\exp\left[-(1-\alpha-\beta)\left(\frac{\partial \ln z_o}{\partial\beta}\right)_{T,V,\alpha}\right] \tag{12}$$

The equation of state for the system is given by

$$P = -\left(\frac{\partial A}{\partial V}\right)_{T,\alpha,\beta}$$

$$= \left(1 + \beta - \frac{\alpha}{2}\right)\frac{MkT}{V}\left[1 + \frac{1 - \alpha - \beta}{1 + \beta - \frac{\alpha}{2}} V \left(\frac{\partial \ln z_o}{\partial V}\right)_{T,\alpha,\beta}\right] \tag{13}$$

where $A = -kT \ln Z$ is the Helmholtz free energy. The second term in the brackets of the right side of equation (13) represents the deviation from the perfect gas law due to the nonzero volume associated with the hydrogen atom. As can be seen from equations (11) and (12), this effect also influences the form of the equations of equilibrium.

Substituting the expressions for z_2, z_H, z_p, and z_e as given by equations (4), (5), (6), and (7), respectively, into equations (11) and (12) and neglecting terms that are second order in the corrections due to the nonzero volume of the hydrogen atoms yield

$$K_1 = \frac{(1 - \beta - \alpha)^2}{\frac{\alpha}{2}\left(1 + \beta - \frac{\alpha}{2}\right)}$$

$$= \frac{(\pi m_H)^{3/2}(kT)^{5/2} z_o^2 \; e^{-q/kT}}{h^3 z_{vr} P}$$

$$= 0.915\times10^{-2} \; \frac{z_o^2 T^{5/2} \; e^{-51.99\times10^3/T}}{z_{vr} P_{atm}} \tag{14}$$

and

$$K_2 = \frac{\beta^2}{(1 - \beta - \alpha)\left(1 + \beta - \frac{\alpha}{2}\right)}$$

$$= \frac{2(2\pi m_e)^{3/2}(m_p/m_H)^{3/2}(kT)^{5/2} \; e^{-I/kT}}{h^3 z_o P}$$

$$= 6.571\times10^{-7} \; \frac{T^{5/2} \; e^{-157.7\times10^3/T}}{z_o P_{atm}} \tag{15}$$

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where K_1 and K_2 are the equilibrium constants based on mole fractions for the dissociation and ionization reactions, respectively.

For given T and P, equations (14) and (15) may be solved simultaneously for α and β. Then, equation (13) is employed to find the value of (V/M), thus defining the equilibrium state of the system completely. The entropy S and enthalpy H of the system result from the application of the thermodynamic relations

$$\frac{S}{M} = -\frac{1}{M}\left(\frac{\partial A}{\partial T}\right)_{V,\alpha,\beta}$$

$$= \frac{k \ln Z}{M} + \frac{kT}{M}\frac{\partial \ln Z}{\partial T}$$

$$= k\left[\ln \frac{(2\pi m_H)^{3/2} k^{5/2}}{h^3} + \ln \frac{1 + \beta - \frac{\alpha}{2}}{1 - \beta - \alpha}\frac{z_o T^{5/2}}{P} + \frac{5}{2}\left(1 + \beta - \frac{\alpha}{2}\right)\right.$$

$$- \frac{\alpha q}{2kT} + \frac{\beta I}{kT} + \frac{\alpha T}{2}\frac{\partial \ln z_{vr}}{\partial T} + (1 - \alpha - \beta)T\frac{\partial \ln z_o}{\partial T}$$

$$\left. - (1 - \alpha - \beta)P\frac{\partial \ln z_o}{\partial P}\right] \tag{16}$$

and

$$\frac{H}{M} = \frac{A + TS + PV}{M}$$

$$= kT\left[\frac{5}{2}\left(1 + \beta - \frac{\alpha}{2}\right) + (1 - \alpha)\frac{q}{2kT} + \frac{\beta I}{kT} + \frac{\alpha T}{2}\frac{\partial \ln z_{vr}}{\partial T}\right.$$

$$\left. + (1 - \alpha - \beta)T\frac{\partial \ln z_o}{\partial T} - (1 - \alpha - \beta)P\frac{\partial \ln z_o}{\partial P}\right] \tag{17}$$

The values resulting from the calculations are given in table I. Over the major portion of the range of pressures (from 10^{-5} to 10^{-1} atm), the dissociation process is complete before the ionization process starts. At higher pressures, overlapping of the two processes occurs, as shown by figure 1. Where no overlapping occurs, either α or β

may be considered to be zero. Also, at the low temperatures and higher pressures, z_o may be taken to have the value 2, thus simplifying the calculations still further.

Where β can be considered to be zero, the fraction of molecules dissociated is given by

$$x = 1 - \alpha$$

$$= \frac{1}{\sqrt{1 + \frac{4}{K_1}}}$$

and, where α can be considered to be zero, the fraction of atoms ionized is given by

$$\beta = \frac{1}{\sqrt{1 + \frac{1}{K_2}}}$$

CONCLUDING REMARKS

Hydrogen gas at equilibrium consists of a collection of diatomic hydrogen molecules, hydrogen atoms, free protons, and free electrons, the relative percentage of each being determined by the particular values of the pressure and temperature. Table I presents equilibrium values of these percentages for hydrogen (75% ortho - 25% para) for temperatures from 300° to 100,000° K and for pressures from 10^{-5} to 10^2 atmospheres. In addition, for these pressure and temperature ranges, the values of specific volume, enthalpy, and entropy are given.

The internal partition function z_{vr} of the diatomic hydrogen molecule is obtained by approximating the forces between the two nuclei by a Morse potential and then applying old quantum-theory considerations to the treatment of the high-energy vibration-rotation levels. Thus, the interdependence of vibrational and rotational motions of the nuclei is taken into account, and the resulting expression is a series that converges more rapidly, the lower the temperature.

Convergence of the internal partition function z_o of the hydrogen atom is obtained as in reference 3 by essentially cutting off the series when the average volume associated with the electronic orbit exceeds the average volume per particle within the gas, and a closed-form expression for z_o that depends on both pressure and temperature is obtained.

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APPENDIX A

APPROXIMATION TO THE INTERNAL PARTITION FUNCTION OF A HYDROGEN MOLECULE

The internal partition function for a hydrogen molecule in normal hydrogen (75% ortho - 25% para) is denoted by z_{vr} and may be expressed in terms of the individual partition functions corresponding to ortho- and parahydrogen:

$$z_{vr} = \frac{3}{4}\left(z_{vr}\right)_{ortho} + \frac{1}{4}\left(z_{vr}\right)_{para} \tag{A1}$$

where $\left(z_{vr}\right)_{ortho}$ is antisymmetric with respect to interchange of the hydrogen nuclei, whereas $\left(z_{vr}\right)_{para}$ is symmetric under this interchange.

At low temperatures, the rotational and vibrational contributions to the partition function may be considered independently. In this case, the possible rotational energy levels are given by

$$\left(\epsilon_{rot}\right)_j = \frac{h^2}{8\pi^2 I} j(j + 1), \quad j = 0,1,2, \ . \ . \ . \tag{A2}$$

where I is the moment of inertia of the molecule about its center of mass. The multiplicity of each level is $(2j + 1)$, and the states corresponding to even values of j are symmetric with respect to nuclei interchange while those corresponding to odd values are antisymmetric. Also, at these low temperatures, the oscillatory motion of the nuclei is small so that, to a good approximation, the potential between the two nuclei can be considered to be a harmonic one. The vibrational energy levels, then, are those of a harmonic oscillator with unit multiplicity and energy values:

$$\left(\epsilon_{vib}\right)_v = h\nu\left(v + \frac{1}{2}\right), \quad v = 0,1,2, \ . \ . \ . \tag{A3}$$

where ν is the characteristic frequency of the vibration. Here, even v-states are symmetric and odd v-states are antisymmetric, and the lowest energy level has the zero-point energy of $h\nu/2$. For the hydrogen molecule, the energy separation of the vibrational levels is about 50 times larger than that of the rotational levels.

When the vibrational and rotational effects can be considered independently, they may be written:

$$(z_{vr})_{ortho} = (z_v)_s(z_r)_a + (z_v)_a(z_r)_s$$

$$(z_{vr})_{para} = (z_v)_s(z_r)_s + (z_v)_a(z_r)_a$$

where the subscripts "s" and "a" denote symmetric and antisymmetric states, respectively. Thus,

$$(z_r)_s = \sum_{j=0,2,4,\ldots} (2j + 1)\, e^{-(\epsilon_{rot})_j/kT}, \qquad (z_r)_a = \sum_{j=1,3,5,\ldots} (2j + 1)\, e^{-(\epsilon_{rot})_j/kT}$$

$$(z_v)_s = \sum_{v=0,2,4,\ldots} e^{-(\epsilon_{vib})_v/kT}, \qquad (z_v)_a = \sum_{v=1,3,5,\ldots} e^{-(\epsilon_{vib})_v/kT}$$

and equation (A1) becomes

$$z_{vr} = (z_v)_a\left[\frac{3}{4}(z_r)_s + \frac{1}{4}(z_r)_a\right] + (z_v)_s\left[\frac{3}{4}(z_r)_a + \frac{1}{4}(z_r)_s\right] \qquad \text{(A4)}$$

As the temperature under consideration increases to room temperature and above, the higher rotational levels start to fill up and the distinction between $(z_r)_s$ and $(z_r)_a$ vanishes. The relations then can be written as

$$\begin{aligned}(z_r)_s &\cong (z_r)_a \\ &\cong \frac{1}{2}\sum_{j=0,1,2,\ldots} (2j + 1)\, e^{-(\epsilon_{rot})_j/kT} \\ &= \frac{z_r}{2}\end{aligned}$$

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and

$$z_r \cong \int_0^\infty (2j + 1)\, e^{-(\epsilon_{rot})_j/kT}\, dj$$

$$= \frac{T}{\Theta_r} \tag{A5}$$

where

$$\Theta_r = \frac{h^2}{8\pi^2 Ik} \tag{A6}$$

Equation (A4) then becomes

$$z_{vr} \cong \left[(z_v)_a + (z_v)_s\right]\frac{z_r}{2}$$

$$= \frac{z_v z_r}{2}$$

$$\cong \frac{T}{2\Theta_r} \sum_{v=0}^{\infty} e^{-(\epsilon_{vib})_v/kT}$$

$$\cong \frac{T}{2\Theta_r} \frac{1}{1 - e^{-\Theta_v/T}} \tag{A7}$$

where

$$\Theta_v = \frac{h\nu}{k} \tag{A8}$$

and the lowest vibration energy level has been taken as the zero level.

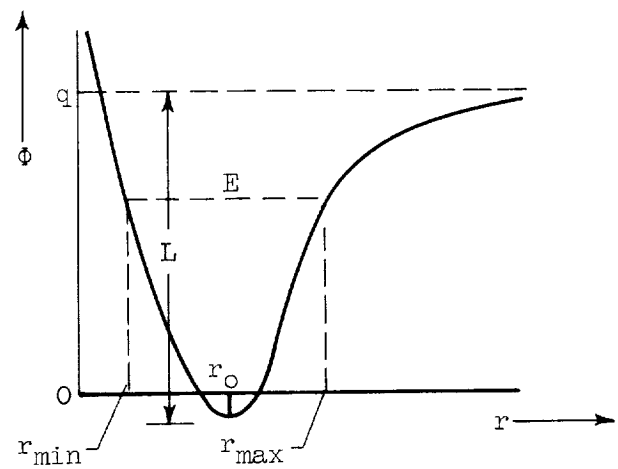
At temperatures above 1000° or 2000° K, the amplitude of the vibrational motion is large, and the approximation that the potential corresponds to that of a harmonic oscillator cannot be made with any degree of accuracy. Also, the interaction between the vibrational and rotational motions must now be taken into account; the vibrational motion increases the distance of separation between the atoms, thus increasing the moment of inertia, which in turn decreases the separation of the

rotational energy levels (eq. (A2)), while the centrifugal forces set up because of the rotational motion affect the oscillatory motion. The following calculations are based on the assumption of a Morse potential between the two nuclei of the molecule, and the stretching of the molecule is handled from the standpoint of the old quantum theory.

It is first shown that the energies of the vibrational levels obtained by experiment agree well with those obtained from calculations which assume that the interaction between the nuclei can be described by the Morse potential function. The form of the Morse potential is

$$\Phi = -L\left[2e^{-a(r-r_o)} - e^{-2a(r-r_o)}\right] + q \tag{A9}$$

where q is the dissociation energy, r is the separation distance, and L, r_o, and a are constants (see sketch). If the old quantum theory is employed,



the number n of vibrational energy levels up to an energy value of E is given by the expression

$$n = \frac{1}{h} \iint dp\, dq$$

$$= \frac{\sqrt{m_H}}{h} \int_{r_{min}}^{r_{max}} dr \int_{\Phi}^{E} \frac{dE}{\sqrt{E - \Phi}}$$

$$= \frac{2\sqrt{m_H}}{h} \int_{r_{min}}^{r_{max}} \sqrt{E - \Phi}\, dr \tag{A10}$$

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Defining η by the relation

$$E = -L(1 - \eta^2) + q, \qquad 0 \leq \eta \leq 1 \tag{A11}$$

it is found that

$$\left.\begin{aligned} r_{min} &= r_o - \frac{\ln(1 + \eta)}{a} \\ r_{max} &= r_o - \frac{\ln(1 - \eta)}{a} \end{aligned}\right\} \tag{A12}$$

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Substituting equations (A9) and (A11) into equation (A10) and letting

$$\zeta = e^{-a(r-r_o)} - 1 \tag{A13}$$

the integral for n becomes

$$\begin{aligned} n &= \frac{2\sqrt{m_H L}}{ah} \int_{-\eta}^{\eta} \frac{\sqrt{\eta^2 - \zeta^2}}{1 + \zeta} d\zeta \\ &= \frac{2\pi\sqrt{m_H L}}{ah} \left(1 - \sqrt{1 - \eta^2}\right) \end{aligned} \tag{A14}$$

This result is based on the old quantum theory which postulates that the energy levels form a continuum and averages over the actual discrete energy levels.

In order to modify equation (A14) to take account of the fact that the levels are actually discrete, the situation may be examined when $|a(r - r_o)| \ll 1$ and the potential Φ reduces to the harmonic potential with additive constant equal to $[-(L - q)]$:

$$\Phi \cong La^2(r - r_o)^2 - (L - q) \tag{A15}$$

From equation (A3), the possible vibrational energy values for the molecule under the influence of this harmonic potential are

$$E_v = h\nu\left(v + \frac{1}{2}\right) - (L - q), \qquad v = 0,1,2, \ . \ . \ . \tag{A16}$$

where

$$\nu = \frac{a}{\pi}\sqrt{\frac{L}{m_H}} \tag{A17}$$

Inasmuch as the zero energy level is taken as the lowest vibrational energy state of the molecule, it is necessary that

$$L - q = \frac{h\nu}{2}$$

Also, when $\eta^2 \ll 1$, equation (A14) should reduce to equation (A16). When $\eta^2 \ll 1$, equation (A14) becomes

$$n \cong \frac{2\pi\sqrt{m_H L}}{ah}\left(\frac{1}{2}\eta^2\right)$$

$$= \frac{1}{h\nu}(E + L - q)$$

or

$$E \cong nh\nu - (L - q)$$

A comparison of the preceding equation with equation (A16) shows that the proper correspondence between n and v is

$$n = v + \frac{1}{2}, \qquad v = 0,1,2, \ . \ . \ . \tag{A18}$$

Thus, $n = 1/2$ corresponds with the appearance of the first level ($v = 0$), $n = 3/2$ with the second level ($v = 1$), and so forth. The appropriate vibrational energy levels for the Morse potential result from inserting equations (A11) and (A18) into equation (A14):

$$E_v = q - L\left[1 - \frac{ah\left(v + \frac{1}{2}\right)}{2\pi\sqrt{m_H L}}\right]^2 \tag{A19}$$

whose result agrees exactly with the quantum mechanical treatment of the Morse potential (ref. 4).

Herzberg (ref. 5) has listed the spectroscopically determined values of the rotational and vibrational energy levels for the hydrogen

molecule up to the vibrational quantum number $v = 14$. The values for the constants affording agreement to 2 percent with the listed data are

$$\left.\begin{aligned} q &= 7.177\times10^{-12}\ \text{erg} \\ L &= 7.619\times10^{-12}\ \text{erg} \\ a &= 1.995\times10^{8}\ \text{cm}^{-1} \end{aligned}\right\} \tag{A20}$$

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The value of q may be compared with the generally accepted value of $36{,}116\ \text{cm}^{-1} = 7.173\times10^{-12}$ erg. Table II lists both the experimental values of the vibrational energy levels and those calculated from equation (A19). The agreement between the experimental and calculated values demonstrates that the Morse potential is suitable for describing the interaction between the two nuclei.

The Morse potential function is now employed to determine z_{vr}. By the old quantum theory, the number M of vibration-rotation states up to an energy E is

$$M = \frac{1}{h^3} \iiint\!\!\iint\!\!\iint dp_r\ dr\ dp_\theta\ d\theta\ dp_\varphi\ d\varphi$$

where the integration in momentum and position variables in spherical coordinates is carried out up to the energy E. For the hydrogen molecule,

$$E = \frac{p_r^2}{m_H} + \frac{p_\theta^2}{m_H r^2} + \frac{p_\varphi^2}{m_H r^2 \sin^2\theta} + \Phi$$

and performing the integration over all variables except r gives

$$M = \frac{8\pi^2}{3h^3}\, m_H^{3/2} \int_{r_{min}}^{r_{max}} (E - \Phi)^{3/2} r^2\ dr$$

Differentiating with respect to the energy yields the density of energy levels ρ as a function of the energy E:

$$\rho = \frac{dM}{dE}$$

$$= \frac{4\pi^2}{h^3} m_H^{3/2} \int_{r_{min}}^{r_{max}} (E - \Phi)^{1/2} r^2 \, dr \tag{A21}$$

Substituting equations (A9), (A11), (A12), and (A13) yields

$$\rho = \frac{4\pi^2 m_H^{3/2} \sqrt{L}}{h^3 a} \int_{-\eta}^{\eta} \frac{\sqrt{\eta^2 - \zeta^2}}{1 + \zeta} \left[r_o - \frac{\ln(1 + \zeta)}{a} \right]^2 d\zeta$$

$$= \frac{4\pi^2 m_H^{3/2} \sqrt{L}}{h^3 a} \left[\pi r_o^2 \left(1 - \sqrt{1 - \eta^2} \right) - \frac{2r_o}{a} F + \frac{1}{a^2} H \right] \tag{A22}$$

where

$$F \equiv \int_{-\eta}^{\eta} \sqrt{\eta^2 - \zeta^2} \, \frac{\ln(1 + \zeta)}{1 + \zeta} \, d\zeta$$

and

$$H \equiv \int_{-\eta}^{\eta} \sqrt{\eta^2 - \zeta^2} \, \frac{\ln^2(1 + \zeta)}{1 + \zeta} \, d\zeta$$

The integrations for F and H can be accomplished in series yielding

$$F = - \sum_{n=2}^{\infty} A_{2n} \eta^{2n} \tag{A23}$$

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where

$$A_{2n} = \frac{\pi}{2^{2n-1}} \frac{(2n - 2)!}{n!(n - 1)!} \sum_{P=0}^{2n-3} \frac{1}{P + 1}$$

$$\cong \frac{\pi}{2^{2n-1}} \frac{(2n - 2)!}{n!(n - 1)!} \left[\ln\left(2n - \frac{3}{2}\right) + 0.578\right] \tag{A24}$$

and

$$H = \sum_{n=2}^{\infty} B_{2n}\eta^{2n} \tag{A25}$$

where

$$B_{2n} = \frac{\pi}{2^{2n-2}} \frac{(2n - 2)!}{n!(n - 1)!} \sum_{P=0}^{2n-4} \frac{1}{P + 2} \sum_{k=0}^{P} \frac{1}{k + 1}$$

$$\cong \frac{\pi}{2^{2n-1}} \frac{(2n - 2)!}{n!(n - 1)!} \left[\ln^2\left(2n - \frac{3}{2}\right) + 1.156 \ln\left(2n - \frac{3}{2}\right) + \frac{1}{2n - \frac{3}{2}} - 1.303\right] \tag{A26}$$

The preceding result for ρ stems from the application of the old quantum theory, which is based on a continuum of energy levels; and although, at the temperatures in question, the rotation levels may be treated as a continuum, the vibration levels cannot be so considered. At energies between the first ($v = 0$) and the second ($v = 1$) vibration level, there exists only one set of rotation levels, all possessing the vibrational quantum number $v = 0$. At energies between the second and third vibration levels, two sets of rotation levels exist, the first being a continuation of the aforementioned set with $v = 0$ and the second possessing the value $v = 1$. These discontinuities that occur at each discrete vibration level must be reflected in the relation for ρ; and as yet equation (A22), being based on the old quantum theory, shows no such discontinuities. Equation (A22) must therefore be corrected, and the modification necessary can be seen by referring to equation (A14), where it is observed that the factor $1 - \sqrt{1 - \eta^2}$ which occurs in the first term of equation (B23) is directly

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proportional to the multiplicity of the vibrational levels. Thus, the appropriate discontinuities can be incorporated in the expression for ρ by making the substitution

$$1 - \sqrt{1 - \eta^2} = \frac{ah}{2\pi\sqrt{m_H L}}(v + 1)$$

in equation (A22):

$$\rho = \frac{4\pi^2}{h^2}\left(\frac{m_H r_o^2}{2}\right)(v + 1) + \frac{4\pi^2 m_H^{3/2}\sqrt{L}}{h^3 a^3}\left(-2r_o aF + H\right) \qquad \text{(A22a)}$$

The first term on the right side of expression (A22a) is just the density of rotational energy levels that would be obtained from the old quantum theory if the distance between the nuclei of the molecule were fixed at $r = r_o$ and the multiplicity of the vibrational energy levels were taken into account. Hence, the remaining terms must yield the change in the density of levels due to the stretching of the molecule.

It still remains to determine the value of r_o that enters in the expression for ρ. If the classical relation is employed that the average of the square of the distance between the nuclei for a state of energy E is given by

$$\overline{r^2}(E) = \int r^2 \frac{dr}{p_r} \Big/ \int \frac{dr}{p_r}$$

where

$$E = \frac{p_r^2}{m_H} + \Phi,$$

there is obtained

$$\overline{r^2} = r_o^2 - \frac{2r_o}{\pi a}\sqrt{1 - \eta^2}\, G + \frac{\sqrt{1 - \eta^2}}{\pi a^2} J \qquad \text{(A27)}$$

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where

$$G \equiv \int_{-\eta}^{\eta} \frac{1}{\sqrt{\eta^2 - \zeta^2}} \frac{\ln(1 + \zeta)}{1 + \zeta} d\zeta$$

$$= \frac{1}{\eta} \frac{dF}{d\eta} \tag{A28}$$

and

$$J \equiv \int_{-\eta}^{\eta} \frac{1}{\sqrt{\eta^2 - \zeta^2}} \frac{\ln^2(1 + \zeta)}{1 + \zeta} d\zeta$$

$$= \frac{1}{\eta} \frac{dH}{d\eta} \tag{A29}$$

The quantities occurring in equation (A27) may be written in series form:

$$\sqrt{1 - \eta^2}\, G = - \sum_{n=1}^{\infty} C_{2n}\eta^{2n}$$

$$= -2.355\ \eta^2 - 1.277\ \eta^4 - 0.883\ \eta^6 - 0.685\ \eta^8 - \ldots \tag{A30}$$

and

$$\sqrt{1 - \eta^2}\, J = \sum_{n=1}^{\infty} D_{2n}\eta^{2n}$$

$$= 1.571\ \eta^2 + 2.650\ \eta^4 + 2.516\ \eta^6 + 2.291\ \eta^8 + \ldots \tag{A31}$$

When $E = 0$, by equation (A11),

$$\eta_0^2 = 1 - \frac{q}{L}$$

$$= 0.0580$$

and

$$\overline{r^2} = R^2$$

where R^2 can be considered to be the average of the square of the distance between the two nuclei at 0° K. The moment of inertia of the hydrogen molecule at low temperatures is directly proportional to the value of R^2 and determines the spacing between the rotational energy levels (eq. (A2)). Experimentally it is found that (ref. 6)

$$I = \frac{m_H}{2} R^2$$

$$= 4.717\times10^{-41} \text{ g-cm}^2 \tag{A32}$$

Substituting this value of $\overline{R^2}$ in equation (A27) for $E = 0$ yields

$$r_o = 0.7234\times10^{-8} \text{ cm}$$

$$r_o^2 = 0.5234\times10^{-16} \text{ cm}^2$$

With this value of r_o, equation (A22a) gives the proper high-energy limiting values. However, at the lowest energy levels, the equation should reduce to

$$\rho = \frac{4\pi^2}{h^2}\left(\frac{m_H R^2}{2}\right)$$

which it does not. The reason is that only the first term of equation (A22a) is a corrected one. Consequently, at low energies, that is, up to an energy value of $E = \frac{h\nu}{2}$, the following expression for ρ was chosen as being more accurate than that given in equation (A22a):

$$\rho = \frac{4\pi^2}{h^2}\left(\frac{m_H \overline{r^2}}{2}\right)$$

$$= \frac{4\pi^2}{h^2}\frac{m_H}{2}\left(r_o^2 - \frac{2r_o}{\pi a}\sqrt{1 - \eta^2}\, G + \frac{1}{\pi a^2}\sqrt{1 - \eta^2}\, J\right),$$

$$0.0580 \leq \eta^2 \leq 0.1144, \qquad 0 \leq E \leq \frac{h\nu}{2} \tag{A22b}$$

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For larger values of η^2, equation (A22a) applies to a sufficient degree of accuracy.

The final expression for z_{vr} can now be written as

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$$z_{vr} = \int_0^q \rho e^{-E/kT}\, dE$$

$$= \frac{1}{4} + \frac{4\pi^2 I_o kT}{h^2} \sum_v e^{-E_v/kT}$$

$$+ \frac{4\pi^2 (m_H L)^{3/2} e^{(L-q)/kT}}{a^3 h^3} \sum_{n=2}^{\infty} (2r_o a A_{2n} + B_{2n}) \left(\frac{kT}{L}\right)^{n+1} I_n(\alpha,\beta)$$

$$+ \frac{2\pi m_H L}{a^2 h^2} e^{(L-q)/kT} \sum_{n=1}^{\infty} (2r_o a C_{2n} + D_{2n}) \left(\frac{kT}{L}\right)^{n+1} I_n(\gamma,\alpha) \qquad \text{(A33)}$$

where

$$I_o = \frac{m_H}{2} r_o^2$$

$$I_n(x,y) = \int_x^y \zeta^n e^{-\zeta}\, d\zeta$$

$$= n!\left(e^{-x} \sum_{P=0}^{n} \frac{x^P}{P!} - e^{-y} \sum_{P=0}^{n} \frac{y^P}{P!}\right)$$

$$\alpha = \frac{0.1144\ L}{kT}, \qquad \beta = \frac{L}{kT}, \qquad \gamma = \frac{L - q}{kT}$$

The experimental values of the vibrational quantum levels are used to calculate the second term on the right side of equation (A33). The first term (1/4) in equation (A33) takes account of the fact that

in the approximation of $(z_r/2)$ by an integral (see eq. (A5)), one-half the contribution of the first level is being neglected. Substituting the values of the constants in equation (A33) gives

$$
\begin{aligned}
z_{vr} = 0.25 &+ 5.436\times10^{-3}\, T \sum_{v} e^{-E_v/kT} \\
&+ 14.1\times10^{-3} T\, e^{3.202\times10^{3}/T} \sum_{n=2}^{\infty} (2r_o a A_{2n} + B_{2n})(0.018118\times10^{-3}\, T)^n I_n \left(\frac{6.313\times10^{3}}{T}, \frac{55.194\times10^{3}}{T}\right) \\
&+ 0.8306\times10^{-3} T\, e^{3.202\times10^{3}/T} \sum_{n=1}^{\infty} (2r_o a C_{2n} + D_{2n})(0.018118\times10^{-3}\, T)^n I_n \left(\frac{3.202\times10^{3}}{T}, \frac{6.313\times10^{3}}{T}\right) \qquad \text{(A34)}
\end{aligned}
$$

Table III lists the values of $(2r_o a A_{2n} + B_{2n})$ for $n = 2$ to 20, and table IV lists $(2r_o a C_{2n} + D_{2n})$ for $n = 1,2,3,$ and 4. Calculated values of z_{vr} are given in table V, and a graph of $T \frac{d(\ln z_{vr})}{dT}$ against T is presented in figure 2.

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APPENDIX B

APPROXIMATION TO THE INTERNAL PARTITION FUNCTION OF A HYDROGEN ATOM

The quantity in question, z_o, is given by the relation

$$z_o = \sum e^{-\epsilon_e/kT} \tag{B1}$$

where ϵ_e is the energy of the electronic orbit and the summation is taken over all possible electronic states.

For a hydrogen atom, the energy is only a function of the principal quantum number "n" of the orbit:

$$(\epsilon_e)_n = I\left(1 - \frac{1}{n^2}\right)$$

where I is the ionization energy, 21.77×10^{-12} erg, and n takes on the values 1,2,3 . . . . The multiplicity associated with each level is $2n^2$, so that

$$z_o = \sum_{n=1}^{\infty} 2n^2 \; e^{-(\epsilon_e)_n/kT}$$

$$= e^{-C/T} \sum_{n=1}^{\infty} 2n^2 \; e^{C/n^2T} \tag{B2}$$

where $C = I/k = 15.77\times10^4$ °K.

This simple method of handling the problem results in an apparent divergence of the expression for z_o. Altman (ref. 3) has taken the dependence on the volume of a state into account by weighting each state with the factor $e^{-PV_{nl}/kT}$ (ref. 3), where V_{nl} is the volume of the electronic state with principal quantum number n and orbital angular

momentum quantum number l. Because the volume is a function of both n and l, the last equation becomes

$$z_o = e^{-C/T} \sum_{n=1}^{\infty} e^{C/n^2T} \sum_{l=0}^{n-1} 2(2l + 1)\, e^{-PV_{nl}/kT} \tag{B3}$$

where $2(2l + 1)$ is the multiplicity of a state designated by the quantum numbers n and l and the value of l ranges from 0 to $(n - 1)$.

Altman now assumes that the volume is independent of l and uses the simple Bohr theory to give an approximate value for V_{nl}. Actually, the effect of considering different volumes for l may be incorporated by taking the following expression for V_{nl}:

$$V_{nl} = \frac{4}{3}\pi(\overline{r^3})_{nl} = \frac{4}{3}\pi \int \Psi_{nl}^{*} r^3 \Psi_{nl}\, d\tau$$

where Ψ_{nl} is the wave function of the electron orbit in hydrogen designated by the quantum numbers n and l. Carrying out the indicated integration over all space gives the relation

$$\begin{aligned} V_{nl} = \frac{4}{3}\frac{\pi n^2 a_o^3}{2^4}\frac{1}{(n + l)!}\Big[&(n + l + 4)! + 16(n + l + 3)!(n - l - 1) \\ &+ 36(n + l + 2)!(n - l - 1)(n - l - 2) \\ &+ 16(n + l + 1)!(n - l - 1)(n - l - 2)(n - l - 3) \\ &+ (n + l)!(n - l - 1)(n - l - 2)(n - l - 3)(n - l - 4)\Big] \end{aligned} \tag{B4}$$

where a_o, the first Bohr radius in hydrogen, has the value of 0.52917×10^{-8} centimeter. This equation shows that the volume of a state varies as n^6 and, hence, the presence of V_{nl} in the exponent of equation (B3) cuts off the sum over n very rapidly. For small values of n, the exponential factor is essentially unity and the sum over l, which shall be denoted by L_n, adds to $(2n^2)$ as it should.

Writing the volume V_{nl} in terms of the quantity

$$\Delta = n - l - \frac{1}{2}$$

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yields the relation

$$V_{n\Delta} = \frac{4}{3}\pi a_o^3 n^2 \Big[n^4 + 3.125\ n^2 + 0.2109 + \Delta(6n^3 + 1.875\ n)$$

$$- \Delta^2(1.5\ n^2 + 0.9375) - 1.5\ n\ \Delta^3 + 0.375\ \Delta^4\Big]$$

where Δ takes on the values $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots, n - \frac{1}{2}$. It can be seen that the main contribution to the summation L_n is given by the terms corresponding to small values of Δ. For small values of Δ and fairly large values of n, the volume $V_{n\Delta}$ may be approximated by the expression

$$V_{n\Delta} = \frac{4}{3}\pi a_o^3 n^6 \left(1 + 6\frac{\Delta}{n} - 1.5\frac{\Delta^2}{n^2} + 3.125\frac{1}{n^2}\right) \tag{B5}$$

If L_n is approximated by an integral and the terms involving n^4 in the expression for $V_{n\Delta}$ are changed so that integration can be performed more conveniently, the result is

$$L_n = \sum_{l=0}^{n-1} 2(2l + 1)e^{-PV_{nl}/kT} = \sum_{\Delta=\frac{1}{2},\frac{3}{2},\ldots,n-\frac{1}{2}} 4(n - \Delta)e^{-PV_{n\Delta}/kT}$$

$$\cong \int_0^n 4(n - \Delta)e^{-PV_{n\Delta}/kT}\, d\Delta \cong \int_0^n 4(n - \Delta)\exp\left[-bn^6\left(1 + 6\frac{\Delta}{n} - 3\frac{\Delta^2}{n^2}\right)\right] d\Delta$$

$$\cong \frac{2}{3}\frac{1}{bn^4}e^{-bn^6}\left(1 - e^{-3bn^6}\right)$$

where $b = \frac{P}{kT}\frac{4}{3}\pi a_o^3$. Because of the fact that an expression incorrect to terms of order n^4 is used for $V_{n\Delta}$, a factor $(1 - 6bn^4)$ added to the preceding relation somewhat reduces the error involved so that

$$L_n \cong \frac{2}{3}\frac{1}{bn^4}e^{-bn^6}\left(1 - e^{-3bn^6}\right)\left(1 - 6bn^4\right) \tag{B6}$$

Substituting equation (A6) into equation (A3) gives

$$z_o \cong e^{-C/T} \sum_{n=1}^{\infty} e^{C/n^2T} \frac{2}{3} \frac{1}{bn^4} e^{-bn^6}\left(1 - e^{-3bn^6}\right)(1 - 6bn^4) \qquad \text{(B7)}$$

Now it must be noted that $C = 157{,}700^\circ$ K and that b is quite small; in particular, it has the value

$$b = 4.555\times10^{-3} \frac{P_{atm}}{T} \qquad \text{(B8)}$$

where P_{atm} is the pressure in atmospheres. At temperatures less than $20{,}000^\circ$ K, the first term of the sum in equation (B7) predominates because of the factor e^{C/n^2T}. The highest pressure considered in this report is 100 atmospheres and the lowest temperature 300° K; therefore, b has the maximum value of about 10^{-3}. With this value of b, L_1 is practically equal to 2 and z_o very nearly has the value 2 in the temperature range below $20{,}000^\circ$ K. At higher temperatures where additional terms other than the first must be considered, b has a value of 10^{-5} or less; and it is necessary to sum up to a value of $n \geqq 6$ in order to get a value for z_o. Hence, in arriving at a simpler expression for the preceding summation, the first term must be left unchanged. The expression for z_o is written in the following form:

$$z_o \cong e^{-C/T}\left[2e^{C/T} + 8e^{C/4T} + \sum_{n=3}^{\infty} e^{C/n^2T} \frac{2}{3} \frac{1}{bn^4} e^{-bn^6}\left(1 - e^{-3bn^6}\right)(1 - 6bn^4)\right]$$

$$\cong e^{-C/T}\left[2e^{C/T} + 8e^{C/4T} + \sum_{n=3}^{\infty} \left(1 + \frac{C}{n^2T}\right) \frac{2}{3} \frac{1}{bn^4} e^{-bn^6}\left(1 - e^{-3bn^6}\right)(1 - 6bn^4)\right]$$

$$\cong e^{-C/T}\left[2\left(e^{C/T} - 1 - \frac{C}{T}\right) + 8\left(e^{C/4T} - 1 - \frac{C}{4T}\right)\right.$$

$$\left. + \sum_{n=1}^{\infty} \left(1 + \frac{C}{n^2T}\right) \frac{2}{3} \frac{1}{bn^4} e^{-bn^6}\left(1 - e^{-3bn^6}\right)(1 - 6bn^4)\right] \qquad \text{(B9)}$$

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Again, employing integral approximations, to a very good degree of accuracy for values of $b \leqq 10^{-4}$, it is found that

$$\left.\begin{aligned}
\sum_{n=1}^{\infty} e^{-bn^6}\left(1 - e^{-3bn^6}\right) &\cong \frac{0.1913}{b^{1/6}} \\
\sum_{n=1}^{\infty} \frac{1}{n^2} e^{-bn^6}\left(1 - e^{-3bn^6}\right) &\cong 0.2934\ b^{1/6} \\
\sum_{n=1}^{\infty} \frac{1}{n^4} e^{-bn^6}\left(1 - e^{-3bn^6}\right) &\cong 0.5908\ \sqrt{b} - 0.1250\ b \\
\sum_{n=1}^{\infty} \frac{1}{n^6} e^{-bn^6}\left(1 - e^{-3bn^6}\right) &\cong 2.420\ b^{5/6} - 1.500\ b
\end{aligned}\right\} \qquad \text{(B10)}$$

Substituting these results into the expression for z_o yields the desired result

$$z_o \cong e^{-C/T}\left[2e^{C/T} + 8e^{C/4T} - 10.08 - 5\,\frac{C}{T} + \frac{0.3939}{\sqrt{b}} + \left(1.613\,\frac{C}{T} - 0.7652\right)\frac{1}{b^{1/6}} - 1.174\,\frac{C}{T}\,b^{1/6}\right] \qquad \text{(B11)}$$

This expression is found to be accurate to about 1 percent or less over the entire range of this investigation when compared with the original expression (B3).

Equation (B11) is the expression on which the calculations of table I are based and is given in the body of the report. It is instructive to investigate whether the values of z_o change significantly if the dependence on l of the volume V_{nl} is ignored and the simple Bohr theory of circular electronic orbits is employed. In this case, equation (B4) becomes

$$V_{nl} = \frac{4}{3}\,\pi a_o^3 n^6 \qquad \text{(B4a)}$$

and carrying out the same steps as before results in the relations

$$z_o = e^{-C/T} \sum_{n=1}^{\infty} e^{C/n^2T} 2n^2 e^{-bn^6}$$

$$z_o \cong e^{-C/T}\left(2e^{C/T} + 8e^{C/4T} - 10.08 - 5\,\frac{C}{T} + \frac{0.5908}{\sqrt{b}} + 1.855\,\frac{C}{T}\,\frac{1}{b^{1/6}}\right) \tag{B12}$$

A comparison of equations (B11) and (B12) shows that the simple Bohr theory results in higher values for z_o, the difference between the two values approaching 50 percent at high temperatures.

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REFERENCES

1. Hilsenrath, Joseph, et al.: Tables of Thermal Properties of Gases. Cir. 564, NBS, Nov. 1, 1955.

2. Sänger-Bredt, I.: The Thermodynamic Properties of Hydrogen and Water as Possible Working Fluids for Nuclear Rockets. Forschungsinstitut für Phys. der Strahlantriebe E.V.(Germany), May 1958.

3. Altman, David: Thermodynamic Properties and Calculated Rocket Performance of Hydrogen to 20,000° K. Rep. 20-106, Jet Prop. Lab., C.I.T., Sept. 3, 1956.

4. Bauer, Ernest, and Wu, Ta-You: Thermal Expansion of a Linear Chain. Phys. Rev., vol. 104, no. 4, Nov. 15, 1956, pp. 914-915.

5. Herzberg, G., and Howe, L. L.: The Lyman Bands of Molecular Hydrogen. Canadian Jour. Phys., vol. 37, no. 5, May 1959, pp. 636-659.

6. Stoicheff, B. P.: High Resolution Raman Spectroscopy of Gases. IX - Spectra of H_2, HD, and D_2. Canadian Jour. Phys., vol. 35, no. 6, June 1957, pp. 730-741.

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TABLE I. - THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(a) P = 0.00001 atm

T, °K	V/M, cm^3/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
300.	0.1222E 10	0.2688E 02	0.1009E 04	0.1000E 01	
500.	0.2036E 10	0.2863E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 10	0.3004E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 10	0.3105E 02	0.3444E 04	1.0000E 00	
1250.	0.5092E 10	0.3186E 02	0.4350E 04	0.9999E 00	
1500.	0.6126E 10	0.3263E 02	0.5414E 04	0.9973E 00	
1750.	0.7386E 10	0.3430E 02	0.8168E 04	0.9637E 00	
2000.	0.1016E 11	0.4079E 02	0.2052E 05	0.7530E 00	
2250.	0.1613E 11	0.5435E 02	0.4934E 05	0.2404E-00	
2500.	0.2006E 11	0.5974E 02	0.6194E 05	0.3032E-01	
2750.	0.2235E 11	0.6076E 02	0.6459E 05	0.4236E-02	
3000.	0.2443E 11	0.6125E 02	0.6601E 05	0.7944E-03	
3250.	0.2647E 11	0.6166E 02	0.6728E 05	0.1913E-03	
3500.	0.2851E 11	0.6202E 02	0.6852E 05	0.5621E-04	
3750.	0.3055E 11	0.6237E 02	0.6975E 05		0.3928E-05
4000.	0.3258E 11	0.6269E 02	0.7099E 05		0.1585E-04
4250.	0.3462E 11	0.6299E 02	0.7224E 05		0.5451E-04
4500.	0.3666E 11	0.6328E 02	0.7350E 05		0.1641E-03
4750.	0.3871E 11	0.6356E 02	0.7483E 05		0.4415E-03
5000.	0.4077E 11	0.6386E 02	0.7628E 05		0.1080E-02
5500.	0.4503E 11	0.6459E 02	0.8010E 05		0.5101E-02
6000.	0.4979E 11	0.6562E 02	0.8724E 05		0.1878E-01
6500.	0.5596E 11	0.6831E 02	0.1028E 06		0.5695E-01
7000.	0.6542E 11	0.7330E 02	0.1366E 06		0.1472E-00
7500.	0.8096E 11	0.8220E 02	0.2014E 06		0.3251E-00
8000.	0.1032E 12	0.9431E 02	0.2953E 06		0.5837E 00
8500.	0.1254E 12	0.1045E 03	0.3793E 06		0.8107E 00
9000.	0.1413E 12	0.1098E 03	0.4254E 06		0.9279E 00
9500.	0.1527E 12	0.1121E 03	0.4463E 06		0.9730E 00
10000.	0.1621E 12	0.1132E 03	0.4570E 06		0.9893E 00
11000.	0.1790E 12	0.1144E 03	0.4700E 06		0.9979E 00
12000.	0.1955E 12	0.1153E 03	0.4804E 06		0.9994E 00
13000.	0.2118E 12	0.1161E 03	0.4904E 06		0.9998E 00
14000.	0.2281E 12	0.1169E 03	0.5003E 06		0.9999E 00
15000.	0.2444E 12	0.1175E 03	0.5101E 06		0.9999E 00
16000.	0.2607E 12	0.1182E 03	0.5200E 06		0.9999E 00
17000.	0.2770E 12	0.1188E 03	0.5299E 06		0.9999E 00
18000.	0.2933E 12	0.1193E 03	0.5397E 06		1.0000E 00
19000.	0.3095E 12	0.1199E 03	0.5496E 06		1.0000E 00
20000.	0.3258E 12	0.1204E 03	0.5595E 06		1.0000E 00
22000.	0.3584E 12	0.1213E 03	0.5792E 06		1.0000E 00
24000.	0.3910E 12	0.1222E 03	0.5989E 06		1.0000E 00
26000.	0.4236E 12	0.1230E 03	0.6186E 06		1.0000E 00
28000.	0.4562E 12	0.1237E 03	0.6383E 06		1.0000E 00
30000.	0.4888E 12	0.1244E 03	0.6581E 06		1.0000E 00
35000.	0.5702E 12	0.1259E 03	0.7074E 06		1.0000E 00
40000.	0.6517E 12	0.1272E 03	0.7567E 06		1.0000E 00
45000.	0.7331E 12	0.1284E 03	0.8060E 06		1.0000E 00
50000.	0.8146E 12	0.1294E 03	0.8553E 06		1.0000E 00
55000.	0.8961E 12	0.1303E 03	0.9046E 06		1.0000E 00
60000.	0.9775E 12	0.1312E 03	0.9539E 06		1.0000E 00
70000.	0.1140E 13	0.1327E 03	0.1052E 07		1.0000E 00
80000.	0.1303E 13	0.1340E 03	0.1151E 07		1.0000E 00
90000.	0.1466E 13	0.1352E 03	0.1250E 07		1.0000E 00
100000.	0.1629E 13	0.1362E 03	0.1348E 07		1.0000E 00

TABLE I. - Continued. THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(b) P = 0.00010 atm

T, °K	V/M, cm³/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
300.	0.1222E 09	0.2461E 02	0.1009E 04	0.1000E 01	
500.	0.2036E 09	0.2636E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 09	0.2777E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 09	0.2878E 02	0.3444E 04	1.0000E 00	
1250.	0.5091E 09	0.2958E 02	0.4347E 04	1.0000E 00	
1500.	0.6115E 09	0.3029E 02	0.5314E 04	0.9991E 00	
1750.	0.7210E 09	0.3122E 02	0.6837E 04	0.9885E 00	
2000.	0.8800E 09	0.3369E 02	0.1153E 05	0.9197E 00	
2250.	0.1234E 10	0.4089E 02	0.2697E 05	0.6535E 00	
2500.	0.1815E 10	0.5134E 02	0.5174E 05	0.2180E-00	
2750.	0.2195E 10	0.5554E 02	0.6264E 05	0.4009E-01	
3000.	0.2434E 10	0.5659E 02	0.6562E 05	0.7860E-02	
3250.	0.2645E 10	0.5709E 02	0.6718E 05	0.1903E-02	
3500.	0.2850E 10	0.5748E 02	0.6849E 05	0.5617E-03	
3750.	0.3054E 10	0.5782E 02	0.6974E 05	0.1939E-03	
4000.	0.3258E 10	0.5814E 02	0.7098E 05	0.7629E-04	
4250.	0.3462E 10	0.5844E 02	0.7222E 05		0.1724E-04
4500.	0.3666E 10	0.5873E 02	0.7347E 05		0.5189E-04
4750.	0.3870E 10	0.5900E 02	0.7473E 05		0.1396E-03
5000.	0.4074E 10	0.5927E 02	0.7603E 05		0.3414E-03
5500.	0.4488E 10	0.5982E 02	0.7892E 05		0.1613E-02
6000.	0.4917E 10	0.6050E 02	0.8287E 05		0.5939E-02
6500.	0.5390E 10	0.6156E 02	0.8950E 05		0.1804E-01
7000.	0.5970E 10	0.6341E 02	0.1020E 06		0.4702E-01
7500.	0.6770E 10	0.6669E 02	0.1259E 06		0.1081E-00
8000.	0.7962E 10	0.7216E 02	0.1684E 06		0.2217E-00
8500.	0.9702E 10	0.8020E 02	0.2348E 06		0.4011E-00
9000.	0.1187E 11	0.8943E 02	0.3155E 06		0.6186E 00
9500.	0.1393E 11	0.9691E 02	0.3846E 06		0.8004E 00
10000.	0.1554E 11	0.1013E 03	0.4275E 06		0.9070E 00
11000.	0.1774E 11	0.1048E 03	0.4635E 06		0.9801E 00
12000.	0.1950E 11	0.1061E 03	0.4788E 06		0.9948E 00
13000.	0.2116E 11	0.1070E 03	0.4899E 06		0.9983E 00
14000.	0.2280E 11	0.1078E 03	0.5001E 06		0.9993E 00
15000.	0.2443E 11	0.1084E 03	0.5101E 06		0.9996E 00
16000.	0.2606E 11	0.1091E 03	0.5200E 06		0.9997E 00
17000.	0.2769E 11	0.1097E 03	0.5298E 06		0.9998E 00
18000.	0.2932E 11	0.1103E 03	0.5397E 06		0.9998E 00
19000.	0.3095E 11	0.1108E 03	0.5496E 06		0.9999E 00
20000.	0.3258E 11	0.1113E 03	0.5594E 06		0.9999E 00
22000.	0.3584E 11	0.1122E 03	0.5792E 06		0.9999E 00
24000.	0.3910E 11	0.1131E 03	0.5989E 06		0.9999E 00
26000.	0.4236E 11	0.1139E 03	0.6186E 06		0.9999E 00
28000.	0.4562E 11	0.1146E 03	0.6383E 06		0.9999E 00
30000.	0.4888E 11	0.1153E 03	0.6580E 06		1.0000E 00
35000.	0.5702E 11	0.1168E 03	0.7073E 06		1.0000E 00
40000.	0.6517E 11	0.1181E 03	0.7566E 06		1.0000E 00
45000.	0.7331E 11	0.1193E 03	0.8059E 06		1.0000E 00
50000.	0.8146E 11	0.1203E 03	0.8552E 06		1.0000E 00
55000.	0.8961E 11	0.1213E 03	0.9046E 06		1.0000E 00
60000.	0.9775E 11	0.1221E 03	0.9539E 06		1.0000E 00
70000.	0.1140E 12	0.1236E 03	0.1052E 07		1.0000E 00
80000.	0.1303E 12	0.1250E 03	0.1151E 07		1.0000E 00
90000.	0.1466E 12	0.1261E 03	0.1250E 07		1.0000E 00
100000.	0.1629E 12	0.1272E 03	0.1348E 07		1.0000E 00

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TABLE I. - Continued. THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(c) P = 0.00100 atm

T, °K	V/M, cm^3/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
500.	0.1222E 08	0.2238E 02	0.1009E 04	0.1000E 01	
500.	0.2036E 08	0.2410E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 08	0.2550E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 08	0.2651E 02	0.3444E 04	1.0000E 00	
1250.	0.5091E 08	0.2731E 02	0.4346E 04	1.0000E 00	
1500.	0.6111E 08	0.2799E 02	0.5283E 04	0.9997E 00	
1750.	0.7154E 08	0.2869E 02	0.6415E 04	0.9964E 00	
2000.	0.8354E 08	0.2983E 02	0.8576E 04	0.9745E 00	
2250.	0.1023E 09	0.3259E 02	0.1449E 05	0.8840E 00	
2500.	0.1394E 09	0.3878E 02	0.2928E 05	0.6312E 00	
2750.	0.1943E 09	0.4682E 02	0.5035E 05	0.2653E-00	
3000.	0.2357E 09	0.5096E 02	0.6216E 05	0.7115E-01	
3250.	0.2623E 09	0.5228E 02	0.6627E 05	0.1860E-01	
3500.	0.2843E 09	0.5286E 02	0.6821E 05	0.5575E-02	
3750.	0.3052E 09	0.5326E 02	0.6964E 05	0.1934E-02	
4000.	0.3257E 09	0.5359E 02	0.7094E 05	0.7622E-03	
4250.	0.3461E 09	0.5390E 02	0.7220E 05	0.3342E-03	
4500.	0.3665E 09	0.5418E 02	0.7344E 05	0.1603E-03	
4750.	0.3870E 09	0.5445E 02	0.7470E 05		0.4415E-04
5000.	0.4073E 09	0.5471E 02	0.7595E 05		0.1080E-03
5500.	0.4483E 09	0.5521E 02	0.7855E 05		0.5101E-03
6000.	0.4897E 09	0.5572E 02	0.8148E 05		0.1878E-02
6500.	0.5325E 09	0.5632E 02	0.8527E 05		0.5704E-02
7000.	0.5787E 09	0.5716E 02	0.9092E 05		0.1488E-01
7500.	0.6319E 09	0.5843E 02	0.1002E 06		0.3436E-01
8000.	0.6984E 09	0.6045E 02	0.1158E 06		0.7172E-01
8500.	0.7874E 09	0.6356E 02	0.1416E 06		0.1372E-00
9000.	0.9104E 09	0.6812E 02	0.1816E 06		0.2416E-00
9500.	0.1075E 10	0.7416E 02	0.2375E 06		0.3892E-00
10000.	0.1274E 10	0.8095E 02	0.3037E 06		0.5634E 00
11000.	0.1652E 10	0.9149E 02	0.4138E 06		0.8433E 00
12000.	0.1910E 10	0.9585E 02	0.4636E 06		0.9533E 00
13000.	0.2102E 10	0.9758E 02	0.4850E 06		0.9848E 00
14000.	0.2275E 10	0.9856E 02	0.4983E 06		0.9942E 00
15000.	0.2441E 10	0.9932E 02	0.5093E 06		0.9973E 00
16000.	0.2605E 10	0.9999E 02	0.5196E 06		0.9985E 00
17000.	0.2769E 10	0.1006E 03	0.5297E 06		0.9991E 00
18000.	0.2932E 10	0.1012E 03	0.5396E 06		0.9993E 00
19000.	0.3095E 10	0.1017E 03	0.5495E 06		0.9995E 00
20000.	0.3258E 10	0.1022E 03	0.5594E 06		0.9996E 00
22000.	0.3584E 10	0.1031E 03	0.5791E 06		0.9997E 00
24000.	0.3910E 10	0.1040E 03	0.5989E 06		0.9997E 00
26000.	0.4236E 10	0.1048E 03	0.6186E 06		0.9998E 00
28000.	0.4562E 10	0.1055E 03	0.6383E 06		0.9998E 00
30000.	0.4887E 10	0.1062E 03	0.6580E 06		0.9998E 00
35000.	0.5702E 10	0.1077E 03	0.7073E 06		0.9999E 00
40000.	0.6517E 10	0.1090E 03	0.7566E 06		0.9999E 00
45000.	0.7331E 10	0.1102E 03	0.8059E 06		0.9999E 00
50000.	0.8146E 10	0.1112E 03	0.8552E 06		0.9999E 00
55000.	0.8960E 10	0.1122E 03	0.9045E 06		1.0000E 00
60000.	0.9775E 10	0.1130E 03	0.9538E 06		1.0000E 00
70000.	0.1140E 11	0.1146E 03	0.1052E 07		1.0000E 00
80000.	0.1303E 11	0.1159E 03	0.1151E 07		1.0000E 00
90000.	0.1466E 11	0.1170E 03	0.1250E 07		1.0000E 00
100000.	0.1629E 11	0.1181E 03	0.1348E 07		1.0000E 00

TABLE I. - Continued. THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(d) P = 0.01000 atm

T, °K	V/M, cm^3/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
300.	0.1222E 07	0.2007E 02	0.1008E 04	0.1000E 01	
500.	0.2036E 07	0.2182E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 07	0.2322E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 07	0.2424E 02	0.3444E 04	1.0000E 00	
1250.	0.5091E 07	0.2505E 02	0.4346E 04	1.0000E 00	
1500.	0.6110E 07	0.2572E 02	0.5273E 04	0.9999E 00	
1750.	0.7136E 07	0.2634E 02	0.6262E 04	0.9989E 00	
2000.	0.8212E 07	0.2706E 02	0.7636E 04	0.9919E 00	
2250.	0.9503E 07	0.2826E 02	0.1020E 05	0.9631E 00	
2500.	0.1145E 08	0.3068E 02	0.1600E 05	0.8755E 00	
2750.	0.1483E 08	0.3522E 02	0.2795E 05	0.6760E 00	
3000.	0.1981E 08	0.4126E 02	0.4533E 05	0.3787E-00	
3250.	0.2449E 08	0.4568E 02	0.5908E 05	0.1496E-00	
3500.	0.2777E 08	0.4764E 02	0.6566E 05	0.5160E-01	
3750.	0.3026E 08	0.4849E 02	0.6871E 05	0.1865E-01	
4000.	0.3246E 08	0.4897E 02	0.7057E 05	0.7544E-02	
4250.	0.3456E 08	0.4932E 02	0.7203E 05	0.3327E-02	
4500.	0.3663E 08	0.4962E 02	0.7336E 05	0.1600E-02	
4750.	0.3868E 08	0.4990E 02	0.7464E 05	0.8289E-03	
5000.	0.4072E 08	0.5016E 02	0.7589E 05	0.4580E-03	
5500.	0.4481E 08	0.5064E 02	0.7843E 05		0.1613E-03
6000.	0.4891E 08	0.5110E 02	0.8105E 05		0.5939E-03
6500.	0.5304E 08	0.5156E 02	0.8393E 05		0.1804E-02
7000.	0.5729E 08	0.5207E 02	0.8740E 05		0.4707E-02
7500.	0.6176E 08	0.5271E 02	0.9202E 05		0.1067E-01
8000.	0.6665E 08	0.5356E 02	0.9867E 05		0.2273E-01
8500.	0.7227E 08	0.5477E 02	0.1066E 06		0.4376E-01
9000.	0.7907E 08	0.5647E 02	0.1236E 06		0.7851E-01
9500.	0.8764E 08	0.5885E 02	0.1458E 06		0.1324E-00
10000.	0.9865E 08	0.6203E 02	0.1767E 06		0.2109E-00
11000.	0.1296E 09	0.7076E 02	0.2665E 06		0.4453E-00
12000.	0.1671E 09	0.7990E 02	0.3735E 06		0.7089E 00
13000.	0.1989E 09	0.8567E 02	0.4453E 06		0.8775E 00
14000.	0.2226E 09	0.8842E 02	0.4822E 06		0.9504E 00
15000.	0.2418E 09	0.8982E 02	0.5025E 06		0.9783E 00
16000.	0.2594E 09	0.9073E 02	0.5165E 06		0.9894E 00
17000.	0.2763E 09	0.9143E 02	0.5261E 06		0.9941E 00
18000.	0.2928E 09	0.9204E 02	0.5367E 06		0.9964E 00
19000.	0.3093E 09	0.9260E 02	0.5490E 06		0.9975E 00
20000.	0.3256E 09	0.9311E 02	0.5591E 06		0.9981E 00
22000.	0.3583E 09	0.9406E 02	0.5790E 06		0.9988E 00
24000.	0.3909E 09	0.9492E 02	0.5988E 06		0.9991E 00
26000.	0.4235E 09	0.9571E 02	0.6185E 06		0.9993E 00
28000.	0.4561E 09	0.9644E 02	0.6383E 06		0.9994E 00
30000	0.4887E 09	0.9712E 02	0.6580E 06		0.9995E 00
35000.	0.5702E 09	0.9864E 02	0.7073E 06		0.9996E 00
40000.	0.6516E 09	0.9996E 02	0.7566E 06		0.9997E 00
45000.	0.7331E 09	0.1011E 03	0.8059E 06		0.9998E 00
50000.	0.8146E 09	0.1022E 03	0.8552E 06		0.9998E 00
55000.	0.8960E 09	0.1031E 03	0.9045E 06		0.9999E 00
60000.	0.9775E 09	0.1040E 03	0.9538E 06		0.9999E 00
70000.	0.1140E 10	0.1055E 03	0.1052E 07		0.9999E 00
80000.	0.1303E 10	0.1068E 03	0.1151E 07		0.9999E 00
90000.	0.1466E 10	0.1080E 03	0.1250E 07		0.9999E 00
100000.	0.1629E 10	0.1090E 03	0.1348E 07		1.0000E 00

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TABLE I. - Continued. THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(e) P = 0.10000 atm

T, °K	V/M, cm³/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
300.	0.1222E 06	0.1785E 02	0.1000E 04	0.1000E 01	
500.	0.2036E 06	0.1955E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 06	0.2099E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 06	0.2197E 02	0.3444E 04	0.1000E 01	
1250.	0.5091E 06	0.2278E 02	0.4346E 04	1.0000E 00	
1500.	0.6110E 06	0.2344E 02	0.5270E 04	1.0000E 00	
1750.	0.7130E 06	0.2404E 02	0.6240E 04	0.9996E 00	
2000.	0.8167E 06	0.2463E 02	0.7339E 04	0.9975E 00	
2250.	0.9271E 06	0.2533E 02	0.8837E 04	0.9863E 00	
2500.	0.1059E 07	0.2640E 02	0.1139E 05	0.9604E 00	
2750.	0.1241E 07	0.2820E 02	0.1615E 05	0.8923E 00	
3000.	0.1519E 07	0.3115E 02	0.2465E 05	0.7568E 00	
3250.	0.1926E 07	0.3522E 02	0.3739E 05	0.5448E 00	
3500.	0.2404E 07	0.3934E 02	0.5125E 05	0.3139E-00	
3750.	0.2824E 07	0.4215E 02	0.6141E 05	0.1512E-00	
4000.	0.3147E 07	0.4365E 02	0.6720E 05	0.6855E-01	
4250.	0.3407E 07	0.4444E 02	0.7045E 05	0.3185E-01	
4500.	0.3637E 07	0.4492E 02	0.7258E 05	0.1566E-01	
4750.	0.3853E 07	0.4528E 02	0.7423E 05	0.8198E-02	
5000.	0.4064E 07	0.4558E 02	0.7566E 05	0.4552E-02	
5500.	0.4477E 07	0.4608E 02	0.7829E 05	0.1636E-02	
6000.	0.4886E 07	0.4651E 02	0.8081E 05	0.6939E-03	
6500.	0.5298E 07	0.4695E 02	0.8350E 05		0.5704E-03
7000.	0.5711E 07	0.4736E 02	0.8629E 05		0.1489E-02
7500.	0.6131E 07	0.4779E 02	0.8944E 05		0.3438E-02
8000.	0.6564E 07	0.4828E 02	0.9323E 05		0.7190E-02
8500.	0.7020E 07	0.4887E 02	0.9806E 05		0.1385E-01
9000.	0.7514E 07	0.4960E 02	0.1045E 06		0.2490E-01
9500.	0.8066E 07	0.5055E 02	0.1132E 06		0.4222E-01
10000.	0.8701E 07	0.5177E 02	0.1251E 06		0.6807E-01
11000.	0.1036E 08	0.5531E 02	0.1625E 06		0.1554E-00
12000.	0.1275E 08	0.6059E 02	0.2233E 06		0.3035E-00
13000.	0.1593E 08	0.6714E 02	0.3052E 06		0.5032E 00
14000.	0.1941E 08	0.7327E 02	0.3879E 06		0.7002E 00
15000.	0.2250E 08	0.7756E 02	0.4490E 06		0.8390E 00
16000.	0.2501E 08	0.8009E 02	0.4890E 06		0.9161E 00
17000.	0.2710E 08	0.8158E 02	0.5130E 06		0.9547E 00
18000.	0.2897E 08	0.8259E 02	0.5308E 06		0.9739E 00
19000.	0.3073E 08	0.8330E 02	0.5444E 06		0.9838E 00
20000.	0.3244E 08	0.8391E 02	0.5563E 06		0.9892E 00
22000.	0.3576E 08	0.8493E 02	0.5777E 06		0.9942E 00
24000.	0.3905E 08	0.8562E 02	0.5981E 06		0.9962E 00
26000.	0.4232E 08	0.8602E 02	0.6181E 06		0.9972E 00
28000.	0.4559E 08	0.8736E 02	0.6380E 06		0.9978E 00
30000.	0.4885E 08	0.8804E 02	0.6578E 06		0.9982E 00
35000.	0.5700E 08	0.8956E 02	0.7072E 06		0.9988E 00
40000.	0.6515E 08	0.9088E 02	0.7565E 06		0.9991E 00
45000.	0.7330E 08	0.9204E 02	0.8058E 06		0.9993E 00
50000.	0.8145E 08	0.9309E 02	0.8551E 06		0.9994E 00
55000.	0.8960E 08	0.9402E 02	0.9044E 06		0.9995E 00
60000.	0.9774E 08	0.9488E 02	0.9538E 06		0.9996E 00
70000.	0.1140E 09	0.9640E 02	0.1052E 07		0.9997E 00
80000.	0.1303E 09	0.9771E 02	0.1151E 07		0.9998E 00
90000.	0.1466E 09	0.9888E 02	0.1250E 07		0.9998E 00
100000.	0.1629E 09	0.9992E 02	0.1348E 07		0.9999E 00

TABLE I. - Continued. THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(f) P = 1.00000 atm

T, °K	V/M, cm^3/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
300.	0.1222E 05	0.1553E 02	0.1000E 04	0.1000E 01	
500.	0.2036E 05	0.1728E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 05	0.1869E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 05	0.1970E 02	0.3444E 04	0.1000E 01	
1250.	0.5091E 05	0.2050E 02	0.4346E 04	1.0000E 00	
1500.	0.6110E 05	0.2117E 02	0.5269E 04	1.0000E 00	
1750.	0.7129E 05	0.2176E 02	0.6227E 04	0.9999E 00	
2000.	0.8153E 05	0.2231E 02	0.7245E 04	0.9992E 00	
2250.	0.9198E 05	0.2285E 02	0.8404E 04	0.9963E 00	
2500.	0.1031E 06	0.2348E 02	0.9913E 04	0.9875E 00	
2750.	0.1158E 06	0.2433E 02	0.1214E 05	0.9658E 00	
3000.	0.1318E 06	0.2555E 02	0.1567E 05	0.9210E 00	
3250.	0.1535E 06	0.2731E 02	0.2117E 05	0.8404E 00	
3500.	0.1833E 06	0.2969E 02	0.2923E 05	0.7142E 00	
3750.	0.2219E 06	0.3255E 02	0.3957E 05	0.5473E 00	
4000.	0.2654E 06	0.3537E 02	0.5049E 05	0.3708E-00	
4250.	0.3071E 06	0.3760E 02	0.5971E 05	0.2259E-00	
4500.	0.3428E 06	0.3910E 02	0.6625E 05	0.1299E-00	
4750.	0.3726E 06	0.4004E 02	0.7057E 05	0.7391E-01	
5000.	0.3986E 06	0.4065E 02	0.7353E 05	0.4291E-01	
5500.	0.4444E 06	0.4140E 02	0.7749E 05	0.1600E-01	
6000.	0.4871E 06	0.4192E 02	0.8046E 05	0.6874E-02	
6500.	0.5286E 06	0.4235E 02	0.8312E 05	0.3335E-02	
7000.	0.5697E 06	0.4273E 02	0.8567E 05	0.1787E-02	
7500.	0.6113E 06	0.4313E 02	0.8856E 05	0.1035E-02	0.1086E-02
8000.	0.6530E 06	0.4350E 02	0.9146E 05	0.6405E-03	0.2273E-02
8500.	0.6953E 06	0.4389E 02	0.9469E 05	0.4174E-03	0.4378E-02
9000.	0.7388E 06	0.4432E 02	0.9842E 05	0.2834E-03	0.7874E-02
9500.	0.7842E 06	0.4480E 02	0.1029E 06		0.1336E-01
10000.	0.8322E 06	0.4536E 02	0.1084E 06		0.2157E-01
11000.	0.9407E 06	0.4682E 02	0.1237E 06		0.4971E-01
12000.	0.1076E 07	0.4891E 02	0.1478E 06		0.1003E-00
13000.	0.1252E 07	0.5181E 02	0.1841E 06		0.1815E-00
14000.	0.1482E 07	0.5555E 02	0.2347E 06		0.2976E-00
15000.	0.1766E 07	0.5989E 02	0.2976E 06		0.4421E-00
16000.	0.2083E 07	0.6422E 02	0.3647E 06		0.5937E 00
17000.	0.2396E 07	0.6788E 02	0.4251E 06		0.7252E 00
18000.	0.2679E 07	0.7060E 02	0.4725E 06		0.8219E 00
19000.	0.2926E 07	0.7247E 02	0.5071E 06		0.8853E 00
20000.	0.3144E 07	0.7377E 02	0.5324E 06		0.9247E 00
22000.	0.3528E 07	0.7544E 02	0.5673E 06		0.9639E 00
24000.	0.3878E 07	0.7656E 02	0.5929E 06		0.9797E 00
26000.	0.4215E 07	0.7745E 02	0.6152E 06		0.9869E 00
28000.	0.4547E 07	0.7822E 02	0.6362E 06		0.9906E 00
30000.	0.4876E 07	0.7893E 02	0.6565E 06		0.9928E 00
35000.	0.5695E 07	0.8047E 02	0.7065E 06		0.9955E 00
40000.	0.6511E 07	0.8179E 02	0.7560E 06		0.9968E 00
45000.	0.7327E 07	0.8295E 02	0.8055E 06		0.9976E 00
50000.	0.8142E 07	0.8400E 02	0.8548E 06		0.9981E 00
55000.	0.8957E 07	0.8494E 02	0.9042E 06		0.9984E 00
60000.	0.9772E 07	0.8579E 02	0.9535E 06		0.9987E 00
70000.	0.1140E 08	0.8732E 02	0.1052E 07		0.9991E 00
80000.	0.1303E 08	0.8863E 02	0.1151E 07		0.9993E 00
90000.	0.1466E 08	0.8979E 02	0.1249E 07		0.9994E 00
100000.	0.1629E 08	0.9083E 02	0.1348E 07		0.9995E 00

TABLE I. - Continued. THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(g) P = 10.00000 atm

T, °K	V/M, cm^3/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
300.	0.1222E 04	0.1328E 02	0.1009E 04	0.1000E 01	
500.	0.2036E 04	0.1801E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 04	0.1642E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 04	0.1743E 02	0.3444E 04	0.1000E 01	
1250.	0.5091E 04	0.1823E 02	0.4346E 04	1.0000E 00	
1500.	0.6110E 04	0.1890E 02	0.5268E 04	1.0000E 00	
1750.	0.7128E 04	0.1949E 02	0.6222E 04	1.0000E 00	
2000.	0.8148E 04	0.2002E 02	0.7215E 04	0.9997E 00	
2250.	0.9175E 04	0.2051E 02	0.8267E 04	0.9988E 00	
2500.	0.1022E 05	0.2101E 02	0.9447E 04	0.9960E 00	
2750.	0.1132E 05	0.2155E 02	0.1087E 05	0.9892E 00	
3000.	0.1253E 05	0.2219E 02	0.1271E 05	0.9749E 00	
3250.	0.1391E 05	0.2299E 02	0.1522E 05	0.9489E 00	
3500.	0.1559E 05	0.2401E 02	0.1867E 05	0.9061E 00	
3750.	0.1769E 05	0.2530E 02	0.2335E 05	0.8415E 00	
4000.	0.2033E 05	0.2687E 02	0.2943E 05	0.7520E 00	
4250.	0.2355E 05	0.2866E 02	0.3681E 05	0.6393E 00	
4500.	0.2726E 05	0.3054E 02	0.4502E 05	0.5125E 00	
4750.	0.3121E 05	0.3230E 02	0.5318E 05	0.3869E-00	
5000.	0.3507E 05	0.3386E 02	0.6046E 05	0.2777E-00	
5500.	0.4184E 05	0.3561E 02	0.7100E 05	0.1322E-00	
6000.	0.4734E 05	0.3692E 02	0.7732E 05	0.6297E-01	
6500.	0.5210E 05	0.3759E 02	0.8152E 05	0.3192E-01	
7000.	0.5652E 05	0.3808E 02	0.8479E 05	0.1745E-01	
7500.	0.6078E 05	0.3847E 02	0.8766E 05	0.1024E-01	
8000.	0.6496E 05	0.3882E 02	0.9034E 05	0.6393E-02	
8500.	0.6919E 05	0.3919E 02	0.9342E 05	0.4187E-02	0.1381E-02
9000.	0.7339E 05	0.3953E 02	0.9635E 05	0.2870E-02	0.2485E-02
9500.	0.7763E 05	0.3987E 02	0.9949E 05	0.2039E-02	0.4219E-02
10000.	0.8195E 05	0.4022E 02	0.1029E 06	0.1492E-02	0.6815E-02
11000.	0.9098E 05	0.4101E 02	0.1112E 06	0.8546E-03	0.1573E-01
12000.	0.1009E 06	0.4198E 02	0.1224E 06		0.3187E-01
13000.	0.1121E 06	0.4319E 02	0.1376E 06		0.5830E-01
14000.	0.1253E 06	0.4473E 02	0.1583E 06		0.9825E-01
15000.	0.1413E 06	0.4664E 02	0.1861E 06		0.1546E-00
16000.	0.1605E 06	0.4893E 02	0.2217E 06		0.2288E-00
17000.	0.1834E 06	0.5158E 02	0.2649E 06		0.3197E-00
18000.	0.2095E 06	0.5436E 02	0.3140E 06		0.4226E-00
19000.	0.2379E 06	0.5713E 02	0.3654E 06		0.5289E 00
20000.	0.2669E 06	0.5968E 02	0.4143E 06		0.6288E 00
22000.	0.3217E 06	0.6359E 02	0.4968E 06		0.7837E 00
24000.	0.3687E 06	0.6605E 02	0.5533E 06		0.8748E 00
26000.	0.4095E 06	0.6762E 02	0.5924E 06		0.9235E 00
28000.	0.4467E 06	0.6873E 02	0.6223E 06		0.9497E 00
30000.	0.4820E 06	0.6960E 02	0.6475E 06		0.9645E 00
35000.	0.5666E 06	0.7130E 02	0.7026E 06		0.9813E 00
40000.	0.6492E 06	0.7267E 02	0.7538E 06		0.9879E 00
45000.	0.7313E 06	0.7385E 02	0.8039E 06		0.9913E 00
50000.	0.8131E 06	0.7490E 02	0.8536E 06		0.9933E 00
55000.	0.8947E 06	0.7584E 02	0.9032E 06		0.9947E 00
60000.	0.9764E 06	0.7671E 02	0.9527E 06		0.9956E 00
70000.	0.1140E 07	0.7823E 02	0.1052E 07		0.9969E 00
80000.	0.1303E 07	0.7955E 02	0.1150E 07		0.9977E 00
90000.	0.1466E 07	0.8071E 02	0.1249E 07		0.9982E 00
100000.	0.1629E 07	0.8175E 02	0.1348E 07		0.9985E 00

TABLE I. - Concluded. THERMODYNAMIC PROPERTIES OF EQUILIBRIUM HYDROGEN

(h) P = 100.00000 atm

T, °K	V/M, cm^3/g	S/M, cal/(g)(°K)	H/M, cal/g	α	β
300.	0.1222E 03	0.1099E 02	0.1008E 04	0.1000E 01	
500.	0.2036E 03	0.1274E 02	0.1696E 04	0.1000E 01	
750.	0.3055E 03	0.1414E 02	0.2562E 04	0.1000E 01	
1000.	0.4073E 03	0.1515E 02	0.3444E 04	0.1000E 01	
1250.	0.5091E 03	0.1595E 02	0.4346E 04	1.0000E 00	
1500.	0.6110E 03	0.1663E 02	0.5268E 04	1.0000E 00	
1750.	0.7128E 03	0.1722E 02	0.6221E 04	1.0000E 00	
2000.	0.8147E 03	0.1774E 02	0.7206E 04	0.9999E 00	
2250.	0.9168E 03	0.1822E 02	0.8224E 04	0.9996E 00	
2500.	0.1020E 04	0.1868E 02	0.9300E 04	0.9987E 00	
2750.	0.1124E 04	0.1912E 02	0.1046E 05	0.9966E 00	
3000.	0.1232E 04	0.1958E 02	0.1177E 05	0.9921E 00	
3250.	0.1345E 04	0.2006E 02	0.1330E 05	0.9838E 00	
3500.	0.1468E 04	0.2061E 02	0.1515E 05	0.9702E 00	
3750.	0.1605E 04	0.2123E 02	0.1740E 05	0.9493E 00	
4000.	0.1761E 04	0.2195E 02	0.2018E 05	0.9193E 00	
4250.	0.1941E 04	0.2277E 02	0.2356E 05	0.8786E 00	
4500.	0.2152E 04	0.2369E 02	0.2762E 05	0.8261E 00	
4750.	0.2396E 04	0.2472E 02	0.3236E 05	0.7616E 00	
5000.	0.2675E 04	0.2582E 02	0.3771E 05	0.6864E 00	
5500.	0.3323E 04	0.2807E 02	0.4954E 05	0.5166E 00	
6000.	0.4025E 04	0.3008E 02	0.6108E 05	0.3530E-00	
6500.	0.4696E 04	0.3161E 02	0.7062E 05	0.2263E-00	
7000.	0.5297E 04	0.3267E 02	0.7779E 05	0.1420E-00	
7500.	0.5834E 04	0.3342E 02	0.8316E 05	0.9017E-01	
8000.	0.6325E 04	0.3396E 02	0.8737E 05	0.5890E-01	
8500.	0.6786E 04	0.3439E 02	0.9091E 05	0.3981E-01	
9000.	0.7235E 04	0.3478E 02	0.9433E 05	0.2777E-01	0.7711E-03
9500.	0.7671E 04	0.3512E 02	0.9743E 05	0.2002E-01	0.1316E-02
10000.	0.8103E 04	0.3543E 02	0.1005E 06	0.1483E-01	0.2134E-02
11000.	0.8966E 04	0.3603E 02	0.1068E 06	0.8727E-02	0.4944E-02
12000.	0.9846E 04	0.3664E 02	0.1138E 06	0.5577E-02	0.1004E-01
13000.	0.1077E 05	0.3730E 02	0.1220E 06	0.3712E-02	0.1842E-01
14000.	0.1175E 05	0.3804E 02	0.1320E 06	0.2564E-02	0.3119E-01
15000.	0.1281E 05	0.3888E 02	0.1442E 06	0.1813E-02	0.4948E-01
16000.	0.1400E 05	0.3984E 02	0.1591E 06	0.1296E-02	0.7441E-01
17000.	0.1532E 05	0.4094E 02	0.1772E 06	0.9281E-03	0.1070E-00
18000.	0.1683E 05	0.4219E 02	0.1991E 06	0.6590E-03	0.1479E-00
19000.	0.1853E 05	0.4358E 02	0.2248E 06	0.4596E-03	0.1976E-00
20000.	0.2045E 05	0.4510E 02	0.2546E 06	0.3114E-03	0.2557E-00
22000.	0.2495E 05	0.4842E 02	0.3242E 06	0.1234E-03	0.3922E-00
24000.	0.3006E 05	0.5208E 02	0.4086E 06		0.5208E 00
26000.	0.3526E 05	0.5494E 02	0.4781E 06		0.6449E 00
28000.	0.4023E 05	0.5719E 02	0.5387E 06		0.7425E 00
30000.	0.4481E 05	0.5889E 02	0.5878E 06		0.8128E 00
35000.	0.5488E 05	0.6160E 02	0.6754E 06		0.9072E 00
40000.	0.6386E 05	0.6331E 02	0.7393E 06		0.9458E 00
45000.	0.7241E 05	0.6463E 02	0.7950E 06		0.9640E 00
50000.	0.8078E 05	0.6573E 02	0.8474E 06		0.9740E 00
55000.	0.8906E 05	0.6671E 02	0.8985E 06		0.9802E 00
60000.	0.9729E 05	0.6758E 02	0.9489E 06		0.9842E 00
70000.	0.1137E 06	0.6912E 02	0.1049E 07		0.9892E 00
80000.	0.1301E 06	0.7045E 02	0.1148E 07		0.9921E 00
90000.	0.1464E 06	0.7162E 02	0.1247E 07		0.9939E 00
100000.	0.1627E 06	0.7266E 02	0.1346E 07		0.9952E 00

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TABLE II. - COMPARISON OF EXPERIMENTALLY MEASURED VALUES OF VIBRATIONAL ENERGY LEVELS OF THE HYDROGEN MOLECULES WITH VALUES AS CALCULATED BY EQUATION (B19)

v	Energy, E_v, cm^{-1}	
	Experimental (ref. 5)	Equation (B19)
0	0	0
1	4,161	4,254
2	8,087	8,241
3	11,782	11,962
4	15,250	15,417
5	18,492	18,605
6	21,506	21,527
7	24,288	24,183
8	26,831	26,573
9	29,124	28,696
10	31,150	30,553
11	32,887	32,144
12	34,302	33,460
13	35,351	34,526
14	35,973	35,318

TABLE III. - VALUES OF CONSTANTS

A_{2n} AND B_{2n}

n	A_{2n}	B_{2n}	$2r_oaA_{2n} + B_{2n}$
2	0.58905	0.3927	2.0652
3	.40906	.5727	1.734
4	.30066	.5536	1.407
5	.23348	.50335	1.166
6	.18871	.4529	.9887
7	.15709	.4083	.8543
8	.13374	.37004	.7497
9	.11587	.33744	.6664
10	.10183	.30955	.5987
11	.090522	.2855	.5425
12	.079434	.26467	.4902
13	.073540	.24644	.4552
14	.067024	.2304	.4207
15	.061461	.2162	.3907
16	.056660	.2035	.3644
17	.052482	.1921	.3411
18	.048816	.1819	.3205
19	.045578	.1726	.3020
20	.042698	.1642	.2854

TABLE IV. - VALUES OF CONSTANTS

C_{2n} AND D_{2n}

n	C_{2n}	D_{2n}	$2r_oaC_{2n} + D_{2n}$
1	2.355	1.571	8.258
2	1.277	2.650	6.268
3	.883	2.516	4.997
4	.685	2.291	4.215

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TABLE V. - CALCULATED VALUES OF z_{vr}

T, °K	z_{vr}	T, °K	z_{vr}	T, °K	z_{vr}
300	2.020	4,750	41.65	18,000	463.9
500	3.213	5,000	45.20	19,000	511.2
750	4.718	5,500	52.81	20,000	560.0
1000	6.214	6,000	61.13	22,000	661.4
1250	7.802	6,500	70.18	24,000	767.3
1500	9.422	7,000	79.96	26,000	877.0
1750	11.125	7,500	90.49	28,000	990.1
2000	12.93	8,000	101.8	30,000	1106
2250	14.84	8,500	113.8	35,000	1406
2500	16.88	9,000	126.5	40,000	1716
2750	19.04	9,500	140.0	45,000	2035
3000	21.34	10,000	154.2	50,000	2359
3250	23.78	11,000	184.8	55,000	2688
3500	26.37	12,000	217.9	60,000	3021
3750	29.11	13,000	253.6	70,000	3694
4000	32.00	14,000	291.7	80,000	4375
4250	35.06	15,000	331.9	90,000	5061
4500	38.27	16,000	374.1	100,000	5751
		17,000	418.1		

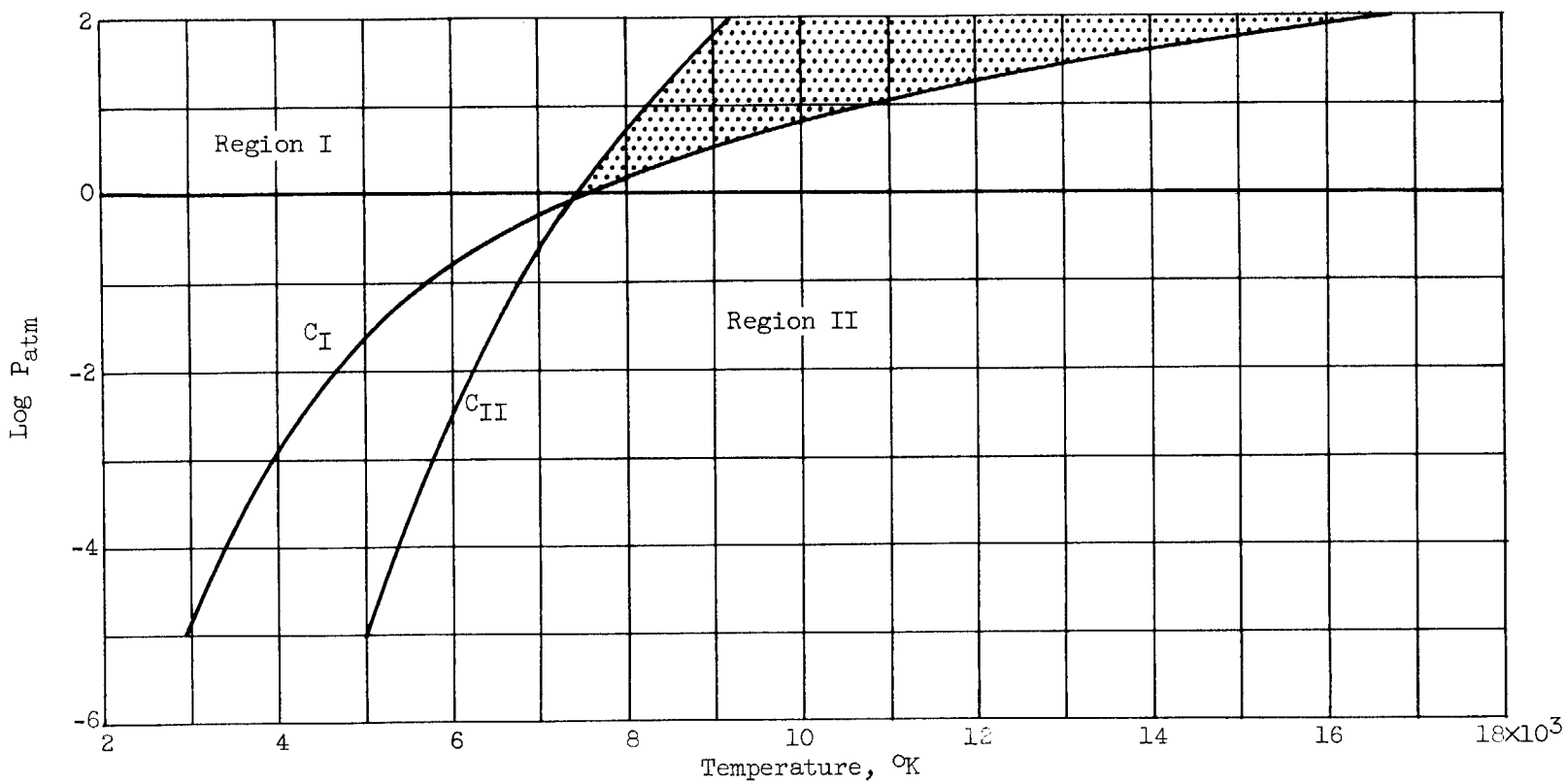

Figure 1. - Illustration of overlap of dissociation and ionization processes at high pressures. Region I with bounding curve, C_I, represents area in which $\alpha \geq 10^{-3}$; region II with bounding curve, C_{II}, is area in which $\beta \geq 10^{-3}$; shaded region is overlap area.

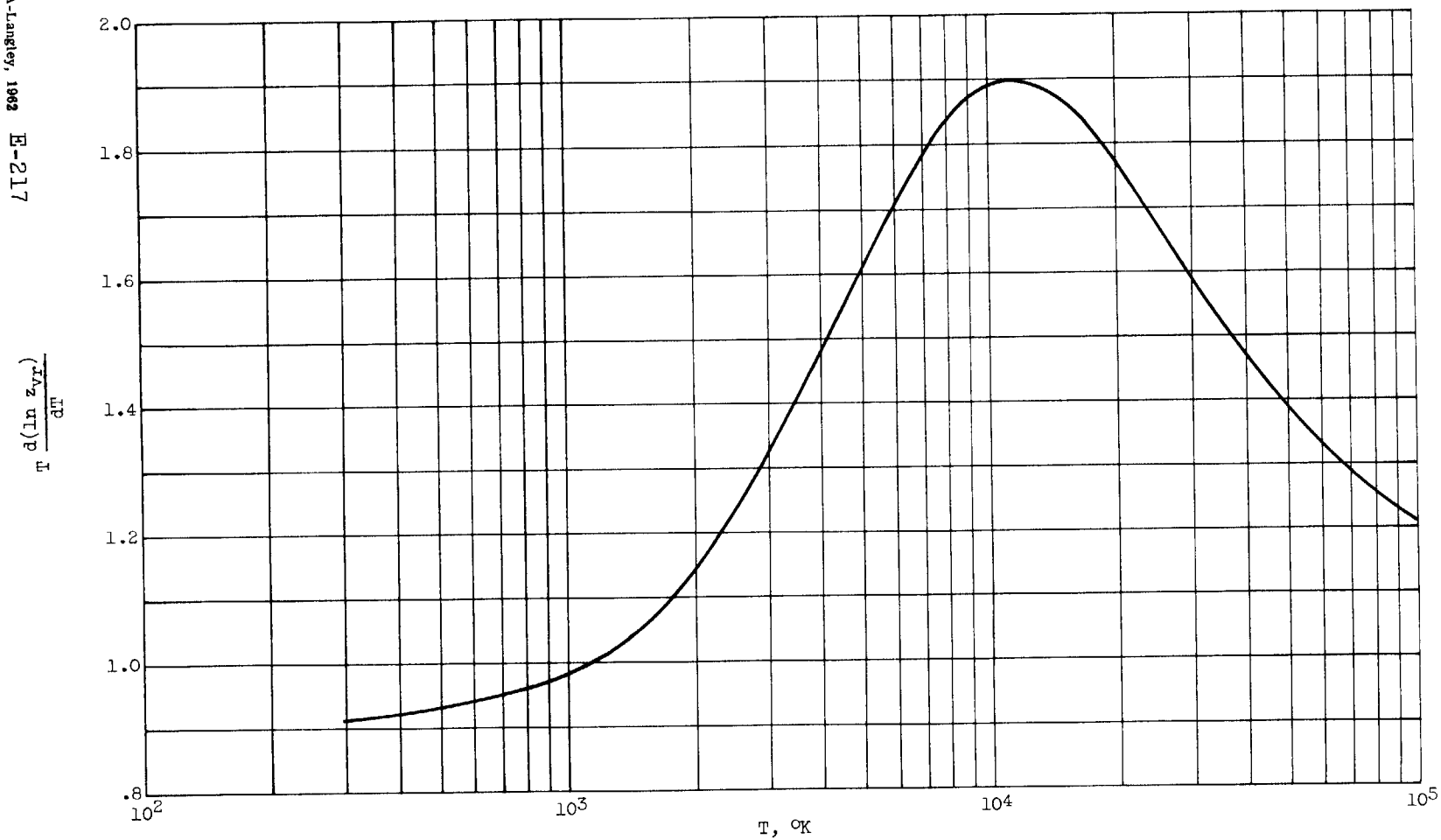

Figure 2. - Plot of $T \frac{d \ln z_{vr}}{dT}$ against T.

NASA-Langley, 1962 E-217