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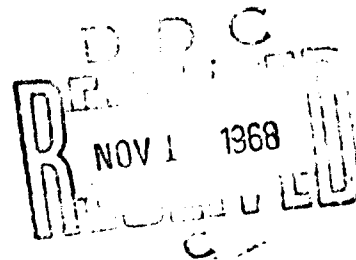
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Theoretical Thermodynamic Properties
of Gases at High Temperatures and Densities
with Numerical Results for Hydrogen

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52

CONTENTS

Abstract	ii
Problem Status	ii
Authorization	ii
INTRODUCTION	1
THE PARTITION FUNCTION	3
THERMODYNAMIC FUNCTIONS	4
HYDROGEN PROPERTIES	5
REFERENCES	6
APPENDIX A - Molecular Potential Correction to Thermodynamic Properties	42
APPENDIX B - Graphs of Selected Thermodynamic Properties of Hydrogen	45

ABSTRACT

The partition function corresponding to an equation of state for a high-temperature, high-density gas suggested by J. S. Rowlinson has been derived. The equations for selected thermodynamic properties of the gas are obtained from this partition function using statistical thermodynamics. These equations are used to calculate results for the case of hydrogen in the range of temperature between 500°K and 3000°K and in the range of density between 1 and 2000 amagats.

PROBLEM STATUS

This is an interim report; work on the problem is continuing.

AUTHORIZATION

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THEORETICAL THERMODYNAMIC PROPERTIES OF GASES AT
HIGH TEMPERATURES AND DENSITIES WITH NUMERICAL
RESULTS FOR HYDROGEN

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INTRODUCTION

An equation of state for high-temperature, high-density gases has been suggested by Rowlinson (1). The partition function corresponding to this equation has been derived, from which has been calculated the hydrogen-gas properties reported here. The significance of this equation of state is that it accounts for the temperature and density dependence of (a) the two-body, intermolecular forces and (b) the volume occupied by the molecules.

An equation of state which includes these effects can be derived in principle from either of two thermodynamic relationships. One, which will be referred to as the pressure equation, comes from the fact that the internal energy of a gas is composed of two parts. The first part is associated with the kinetic energy which is independent of intermolecular forces and corresponds to the ideal gas term. The second part is associated with the intermolecular forces and depends on the radial distribution function of the gas molecules $g(r)$ and the molecular potential $\psi(r)$ or intermolecular forces $-d\psi(r)/dr$. This pressure equation is (2)

$$p_c^{\ddagger} = RT - \frac{N_0^2}{6v} \int_0^{\infty} g(r) \frac{d\psi(r)}{dr} 4\pi r^3 dr, \quad (1)$$

where N_0 is Avogadro's number.

The second relationship from which one can obtain an equation of state for a real gas was developed by Ornstein and Zernike (3) and will be referred to as the compressibility equation:

$$-\frac{RT}{v^2} \left(\frac{v}{p} \right) = 1 + \frac{N_0}{v} \int_0^{\infty} [g(r) - 1] 4\pi r^3 dr, \quad (2)$$

Both equations make the assumptions that (a) all intermolecular forces are two-body forces only, (b) the intermolecular potential is spherically symmetric and, therefore, only a function of radial distance, and (c) classical mechanics applies. The radial distribution function, if correct, should yield the same result from both Eqs. (1) and (2). This agreement has not been possible to achieve, because an exact solution requires the consideration of three-body interactions. Percus and Yevick (4) have suggested an approximation in which three-body interactions are taken in pairs. Using the Percus-Yevick equation, Thiele (5) has obtained, from Eqs. (1) and (2), respectively, the following two equations of state for a gas of hard spheres, i.e., molecules with a square-well potential:

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‡The lower case symbols v , s , h , c , c_p , and ν are quantities per unit mole.

$$\frac{Pv}{RT} = \frac{1 + 2\xi_m + 3\xi_m^2}{(1 - \xi_m)^2} \quad (3)$$

and

$$\frac{Pv}{RT} = \frac{1 + \xi_m + \xi_m^2}{(1 - \xi_m)^3} \quad (4)$$

where $\xi_m = b_m/4v$, in which $b_m = (2/3)\pi N_0 r_m^3$, is related to the volume occupied by the molecules, with r_m being the molecular radius. Thiele observes that Eq. (4) gives a somewhat better result than Eq. (3). The "exact," machine-calculated results lie between the two. Both equations fail near the density of close packing, since no phase transition is predicted.

Rowlinson has extended Thiele's work to the case of a compressible molecule by replacing the square-well potential with the Lennard-Jones $(n/2, n)$ potential:

$$\varphi(r) = \epsilon \left[\left(\frac{r_m}{r} \right)^n - 2 \left(\frac{r_m}{r} \right)^{n/2} \right] \quad (5)$$

where $-\epsilon$ is the minimum value of φ at $r = r_m$. Rowlinson chooses to solve Eq. (2), since according to Thiele it leads to better results than Eq. (1), by equating the integrals with the square-well potential to those with the Lennard-Jones potential on the assumption that the temperature is sufficiently high, i.e., $T > 12\epsilon/k$. The equations will then define σ_x , the equivalent nondimensionalized, hard-sphere radius, and will have the form

$$\int_0^{\sigma_x} (-1) \rho^{\kappa-1} d\rho = \int_0^{\infty} \left[e^{-\varphi(\rho)/kT} - 1 \right] \rho^{\kappa-1} d\rho \quad (6)$$

where $\rho = r/r_m$ and κ is an exponent in the range $0 < \kappa < n/2$. Rowlinson has shown that if a suitable expansion of the right side of Eq. (6) is made with the variable $x = \epsilon/kT$ and if terms greater than the order $1/n$ are neglected, then σ_x is independent of κ and is given by

$$\sigma = \frac{r}{r_m} = x^{1/n} \left[1 + \frac{1}{n} F(x) \right] \quad (7)$$

where

$$F(x) = \gamma_e - 2\sqrt{\pi x} \sum_{l=0}^{\infty} \frac{x^l}{(2l+1)l!} - \sum_{m=1}^{\infty} \frac{(m-1)! 2^{2m} x^m}{(2m)!} \quad (8)$$

in which γ_e is Euler's constant. The fixed radius of a rigid sphere can now be replaced by the variable radius $r = r_m \sigma$, so that b can be substituted for b_m and ξ for ξ_m ; therefore,

$$\xi = \frac{b}{4v} = \frac{1}{4v} \left(\frac{2}{3} \pi N_0 r^3 \right) = \frac{1}{4v} \left(\frac{2}{3} \pi N_0 r_m^3 \sigma^3 \right)$$

Since $(2/3)\pi N_0 r_m^3 = b_m$ and using Eq. (7) to eliminate σ , then

$$\xi = \frac{b_m}{4v} x^{1-n} \left[1 + \frac{1}{n} F(x) \right]^3 \quad (9)$$

The equation of state is given either by Eq. (3) or (4) with ξ_m replaced by ξ .

Choosing n as 12 gives the usual Lennard-Jones [6, 12] potential and

$$\xi = \frac{b_m}{4v} x^{1-4} \left[1 + \frac{1}{12} F(x) \right]^3 \quad (10)$$

By specifying the equation of state of a gas, the various thermodynamic properties are specified. Commonly used thermodynamic relationships involve the derivatives of these properties with respect to the state variables (P, v, T), however, and must therefore be integrated. For an equation of state such as Eq. (3) or (4), these integrals would be difficult or even impossible to solve analytically.

A more satisfactory approach was found through the use of statistical thermodynamics which related all properties, including the equation of state, to derivatives of a total partition function Q . The relationship for the equation of state is

$$\frac{Pv}{RT} = v \left(\frac{\partial}{\partial v} \ln Q \right)_{T, N, \xi} \quad (11)$$

By substituting either Eq. (3) or (4) for Pv/RT , Eq. (11) can be integrated to yield an analytic expression for those terms of the partition function which depend on v . From this result, the contribution of the intermolecular forces to the thermodynamic properties of interest can be determined (see Appendix A).

THE PARTITION FUNCTION

The total partition function is composed of factors, each of which is associated with a particular type of energy of the gas molecule. To construct the total partition function, the appropriate component partition functions corresponding to independent energy modes are simply multiplied together. In this way the equations are easily altered for different types of molecules (e.g., monatomic and diatomic) or to account for phenomena at different energies of interest (e.g., rotation-vibration or electronic excitations). For a diatomic gas between 500°K and 3000°K and between 1 amagat and 2000 amagats, the total partition function is composed of the following energy-related factors (dissociation and ionization are considered to be negligible in this range):

translational:

$$Q_t = \frac{v}{h^3} (2\pi mkT)^{3/2} \quad (12)$$

potential:

$$Q_p = (1 - \xi) e^{-3\xi(2-\xi)} (1-\xi)^2 \quad (13)$$

rotational - vibrational:

$$Q_{rv} = \sum_{n=0}^{n_{max}} \left(\sum_{\substack{j \\ (\dots)}} (2j+1) e^{-\epsilon_j} j^2 kT + 3 \sum_{\substack{j \\ (\dots)}} (2j+1) e^{-\epsilon_j} j^2 kT \right) \quad (14)$$

where Q_i is the usual partition-function term for an ideal gas; Q_p is the factor due to the intermolecular forces as obtained by integrating Eq. (11), with Eq. (4) as the equation of state, i.e., for $Pv/RT = (1 + \xi + \xi^2)/(1 - \xi)^3$; Q_{rv} is the standard quantum mechanical term for rotation-vibration effects including that of para-hydrogen and ortho-hydrogen; $\epsilon_{j,n}$ is the energy level of the molecule and includes both anharmonicity in the vibration and rotation-vibration interaction; $\epsilon_{j,n}/k$ is given by

$$\left(n + \frac{1}{2}\right) \left\{ 1 - \left(n + \frac{1}{2}\right) \left[x_v - \left(n + \frac{1}{2}\right) y_v \right] \right\} \theta_{v,n} - \left(n + \frac{1}{2}\right) j(j+1) a_j' \\ + (j+1) [B_j' - (j+1)(D_j' - (j+1)H_j')],$$

where $\theta_{v,n}$, a_j' , B_j' , D_j' , and H_j' are the usual constants characteristic of the gas multiplied by hc/k ; and n_{max} is the quantum number of the maximum vibrational energy level due to dissociation. The total partition function for N_0 indistinguishable particles is $Q_{tot} = Q_p^N N_0!$ where $Q = Q_i Q_p Q_{rv}$.

THERMODYNAMIC FUNCTIONS

Having specified the total partition function, it is now possible to obtain any thermodynamic function using fundamental statistical thermodynamic relationships. Those functions of particular interest are the compressibility, the specific internal energy, the specific enthalpy, the specific entropy, the specific heat capacities at constant volume and pressure, and the sound speed. They are given, respectively, by the following equations:

$$\frac{Pv}{RT} = v \left(\frac{\partial \ln Q}{\partial v} \right)_T = Z. \quad (15)$$

$$\frac{u}{RT} = \left(\frac{\partial \ln Q}{\partial \ln T} \right)_v = \frac{3}{2} + \phi(Z-1) + DQ_{rv}. \quad (16)$$

$$\frac{h}{RT} = \frac{u}{RT} + \frac{Pv}{RT} = \frac{u}{RT} + Z. \quad (17)$$

$$\frac{s}{R} = \frac{u}{RT} + \ln \frac{Q}{N_0} + 1. \quad (18)$$

$$\frac{c_v}{R} = \frac{1}{R} \left(\frac{\partial u}{\partial T} \right)_v = \frac{3}{2} + \phi(Z-1) \left(1 + D\phi - \frac{\phi Z Z'}{Z-1} \right) - DQ_{rv} (2 - DQ_{rv}) + D^2 Q_{rv}. \quad (19)$$

$$\frac{c_p}{R} = \frac{c_v}{R} + \frac{1}{R} \left[P + \left(\frac{\partial u}{\partial v} \right)_T \right] \left(\frac{\partial v}{\partial T} \right)_p = \frac{c_v}{R} + \frac{Z(1 - \phi Z')^2}{(1 + Z')}. \quad (20)$$

$$a^2 = - \frac{v^2}{m} \left(\frac{\partial P}{\partial v} \right)_s = -\gamma \frac{v^2}{m} \left(\frac{\partial P}{\partial v} \right)_p = Z(1 + Z') \left(\frac{\gamma RT}{m} \right). \quad (21)$$

where

$$\gamma = \frac{1}{4} \left[1 + \frac{x}{\left(1 + \frac{F}{12} \right)} \frac{dF}{dx} \right]. \quad (22)$$

$$Z' = \frac{\xi}{Z} \left(\frac{dZ}{d\xi} \right) \quad (23)$$

and D and D^2 are operators defined by

$$Df = \frac{T}{f} \left(\frac{df}{dT} \right) \text{ and } D^2f = \frac{T^2}{f} \left(\frac{d^2f}{dT^2} \right) \quad (24)$$

HYDROGEN PROPERTIES

The following properties of hydrogen gas, using Eq. (4) for the equation of state as suggested by Rowlinson, have been evaluated as a function of density ($1 \leq \rho \leq 2000$ amagats) and temperature ($500^\circ\text{K} \leq T \leq 3000^\circ\text{K}$): pressure P , compressibility Z , specific heat capacities at constant volume c_v and constant pressure c_p , sound speed a , specific internal energy u , specific enthalpy h , and specific entropy s . The latter three quantities are presented as relative to their values at $\rho = 1$ amagat and $T = 273.16^\circ\text{K}$, which are denoted as u_0 , h_0 , and s_0 , respectively.

The upper limit on density has been selected so as not to approach too closely the close-packing density given by $\xi_{\text{max}} = \pi \sqrt{2} \sigma = 0.74$ (Ref. 5). For $500^\circ\text{K} \leq T \leq 3000^\circ\text{K}$, this would mean that $3300 \leq \rho_{\text{max}} \leq 4300$ amagats. The upper limit on temperature has been selected so as to avoid any significant molecular dissociation, and the lower limit on temperature is set by the approximation in the theory that $T > n\epsilon/k \approx 450^\circ\text{K}$. Table 1 is a listing of the constants used in the calculations and their sources. The properties of hydrogen are presented in Tables 2 and 3. The temperature and density intervals in these two tables have been chosen so that the error using linear interpolation will be less than 0.1% in almost all cases, with the exception of relative entropy in the vicinity of zero.

A comparison of these results (6) with other published equation of state data for hydrogen (7), (8), (9) shows close agreement. Divergences appear only at the higher end of the density range. For the purpose of this comparison, a value of $S_0/R = 16.866$ from Ref. 7 was used with Ref. 9 and a value of $S_0/R = 15.402$ was used with Ref. 8.

Table 4 gives a breakdown of the contribution to u , h , s , c_v , and c_p from each of the three factors in the partition function. In particular the contribution from the intermolecular potential shows the extent of the deviation from an ideal gas.

Selected graphs of the data from Tables 2 and 3 are presented in Figs. 1 through 7 and in Appendix B. The constant entropy data was calculated using Eq. (18) from which the entropy s_1 for any gas state may be calculated. Any other state s_2 with the same entropy may be obtained by specifying one of the state variables and iterating Eq. (18) for the other state variable until $s_1 = s_2$.

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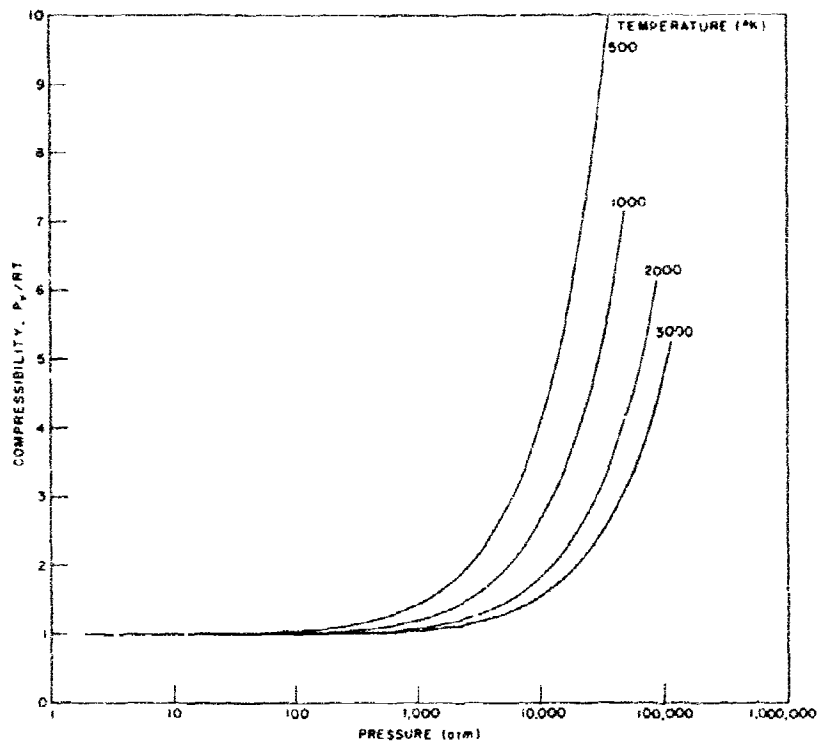


Fig. 1 - Compressibility vs pressure for constant temperature

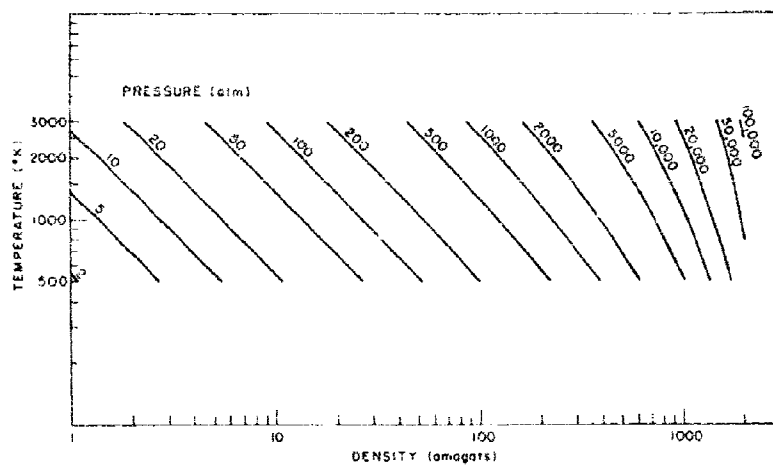


Fig. 2 - Temperature vs density for constant pressure

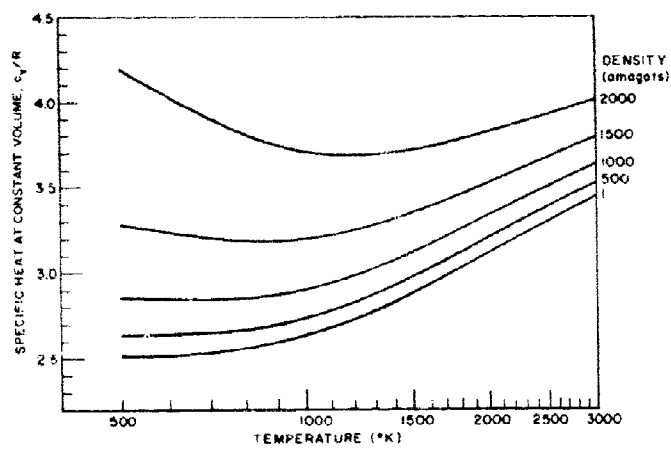


Fig. 3 - Specific heat at constant volume vs temperature for constant density

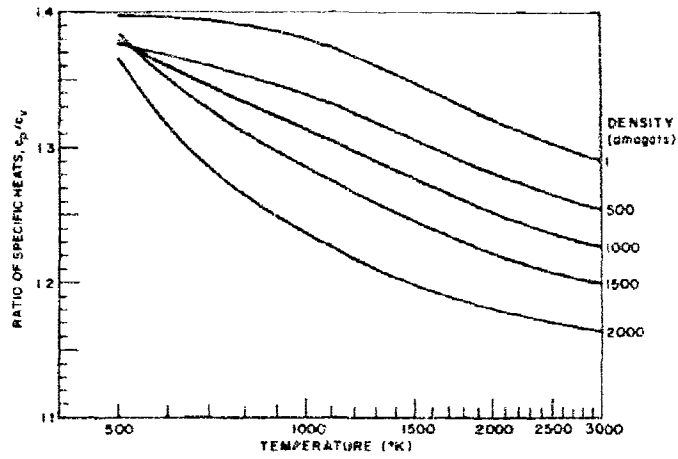


Fig. 4 - Ratio of specific heats vs temperature for constant density

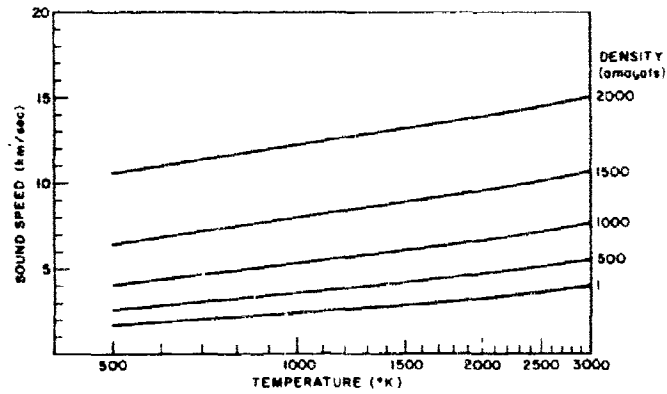


Fig. 5 - Sound speed vs temperature for constant density

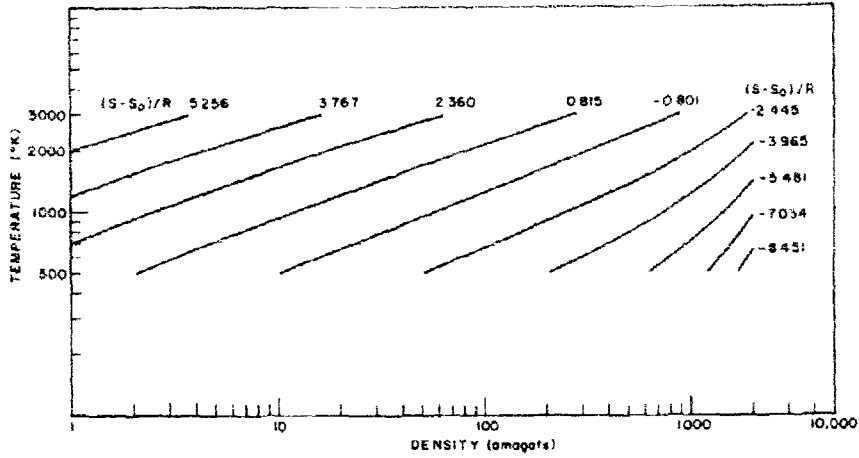


Fig. 6 - Temperature vs density for constant entropy

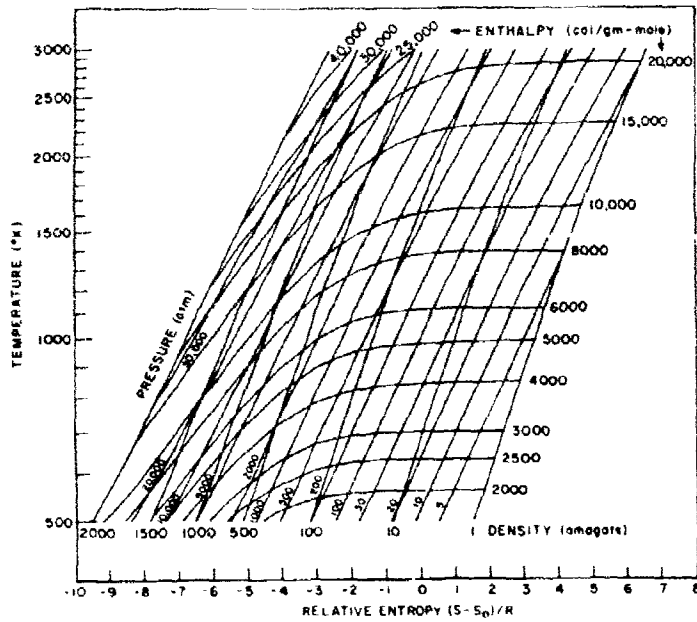


Fig. 7 - Temperature vs relative entropy for constant pressure, density, and enthalpy

Table 1
Hydrogen Constants

Constant	Value	Ref.	Page
R	0.8317×10^{-2} joules/ $^{\circ}$ K/kg-mole or 1.9869 cal/ $^{\circ}$ K/g-mole	10	3437
m	2.016 kg/kg-mole	10	582
N_0	6.0248×10^{23} /mole	10	3437
r_0	2.928×10^{-8} cm	11	1110
$r_m = 2^{1/6} r_0$	3.287×10^{-8} cm	—	—
$b_m = (2/3)\pi N_0 r_m^3$	44.795 cm ³	—	—
ϵ/k	37 $^{\circ}$ K	11	1110
γ_e	0.577215665	10	12
θ_{0e}	6315.5 $^{\circ}$ K	12	468
α_e	3.0664/cm	14	352
B_e	60.848/cm	14	352
D_e	0.04644/cm	14	352
H_e	0.0000497/cm	13	109
$\alpha'_e = hc\alpha_e/k$	4.411 $^{\circ}$ K	—	—
$B'_e = hcB_e/k$	87.54 $^{\circ}$ K	—	—
$D'_e = hcD_e/k$	0.06681 $^{\circ}$ K	—	—
$H'_e = hcH_e/k$	0.0000715 $^{\circ}$ K	—	—
n_{max}	14	—	—
α_e	0.02603	12	468
y_e	0.0000667	13	532
hc/k	1.4388 cm- $^{\circ}$ K	10	3437

Table 2 (Continued)

TEMPERATURE (DEGREE K)	DENSITY (GRAMS/CM ³)										
	300.	350.	400.	450.	500.	600.	700.	800.	900.	1000.	
500.	P(ATH) 729.94 Z 1.3228 Cv/R 2.9434 Cp/R 3.5466 Cp/Cv 1.3806 A(KPS) 2.2033	888.98 1.3864 2.9963 3.5867 1.3791 2.3012	1067.8 1.4589 2.8100 3.5986 1.3786 2.4038	1261.3 1.5322 2.6246 3.6344 1.3771 2.5104	1473.5 1.6109 2.6400 3.8340 1.3765 2.6222	1957.6 1.7037 2.6730 3.6789 1.3759 2.6616	2534.9 1.9795 2.7119 3.7319 1.3761 3.1248	3222.7 2.2021 2.7451 3.7934 1.3761 3.4428	4043.2 2.4557 2.8041 3.8644 1.3761 3.7291	5022.7 2.7457 2.8598 3.9496 1.3766 4.0781	
600.	P(ATH) 867.29 Z 1.3169 Cv/R 2.5894 Cp/R 3.5601 Cp/Cv 1.3748 A(KPS) 2.3989	1061.2 1.3812 2.6019 3.9712 1.3720 2.5030	1272.7 1.4494 2.6151 3.5841 1.3709 2.6119	1503.3 1.5218 2.6290 3.5985 1.3688 2.7252	1794.6 1.5986 2.6437 3.6144 1.3672 2.8437	2327.5 1.7070 2.6759 3.6319 1.3647 3.0970	3007.8 1.9574 2.7120 3.6662 1.3629 3.3747	3816.8 2.1734 2.7527 3.7478 1.3615 3.6772	4779.0 2.4489 2.7986 3.8074 1.3604 4.0096	5924.5 2.6888 2.8506 3.8795 1.3595 4.3747	
700.	P(ATH) 1007.3 Z 1.3110 Cv/R 2.6013 Cp/R 3.5632 Cp/Cv 1.3698 A(KPS) 2.5757	1231.6 1.3739 2.6133 3.5723 1.3669 2.6852	1475.8 1.4408 2.6268 3.5828 1.3643 2.7993	1741.7 1.5112 2.6394 3.5949 1.3620 2.9183	2031.1 1.5882 2.6535 3.6084 1.3598 3.0425	2689.5 1.7501 2.6883 3.6240 1.3561 3.3074	3469.5 1.9332 2.7187 3.6779 1.3520 3.5933	4373.9 2.1445 2.7572 3.7223 1.3500 3.9120	5490.5 2.3820 2.8005 3.7734 1.3475 4.2571	6782.3 2.6521 2.8492 3.8222 1.3450 4.6352	
800.	P(ATH) 1146.2 Z 1.3054 Cv/R 2.6218 Cp/R 3.5773 Cp/Cv 1.3645 A(KPS) 2.7373	1400.3 1.3669 2.6254 3.5847 1.3613 2.8053	1676.7 1.4321 2.6456 3.5939 1.3583 2.9701	1977.1 1.5011 2.6572 3.6037 1.3555 3.0939	2303.6 1.5742 2.6722 3.6133 1.3529 3.2229	3045.2 1.7340 2.6752 3.6244 1.3489 3.3884	3921.4 1.9139 2.7357 3.6583 1.3468 3.6719	4957.2 2.1171 2.7712 3.6874 1.3442 4.0615	6182.5 2.3470 2.8122 3.7563 1.3404 4.4790	7622.9 2.6078 2.8501 3.8171 1.3368 4.8680	
900.	P(ATH) 1284.2 Z 1.3000 Cv/R 2.6523 Cp/R 3.6021 Cp/Cv 1.3586 A(KPS) 2.8862	1567.7 1.3603 2.6262 3.6082 1.3551 3.0043	1875.7 1.4241 2.6749 3.6156 1.3519 3.1272	2210.1 1.4916 2.6870 3.6244 1.3489 3.2551	2573.3 1.5630 2.7001 3.6344 1.3460 3.3884	3395.9 1.7188 2.7285 3.6583 1.3408 3.6719	4385.6 1.8940 2.7601 3.6874 1.3368 4.0615	5509.2 2.0914 2.7951 3.7218 1.3315 4.4790	6850.4 2.3143 2.8342 3.7617 1.3273 4.8680	8451.2 2.5666 2.8777 3.8073 1.3230 5.2708	
1000.	P(ATH) 1421.4 Z 1.2950 Cv/R 2.6890 Cp/R 3.6361 Cp/Cv 1.3522 A(KPS) 3.0264	1734.0 1.3541 2.7000 3.6412 1.3486 3.1460	2073.1 1.4166 2.7115 3.6479 1.3452 3.2726	2443.0 1.4826 2.7256 3.6550 1.3420 3.4043	2840.1 1.5525 2.7364 3.6638 1.3389 3.5413	3742.2 1.7047 2.7648 3.6849 1.3333 3.8329	4803.3 1.8755 2.7942 3.7169 1.3280 4.1484	6051.5 2.0675 2.8279 3.7417 1.3231 4.4915	7520.6 2.2839 2.8653 3.7776 1.3184 4.8645	9250.7 2.5284 2.9088 3.8186 1.3137 5.2708	
1200.	P(ATH) 1693.7 Z 1.2890 Cv/R 1.7811 Cp/R 3.7230 Cp/Cv 1.3460 A(KPS) 3.2750	2063.6 1.3429 2.7918 3.7267 1.3349 3.4029	2464.6 1.4031 2.8024 3.7353 1.3313 3.5358	2897.0 1.4666 2.8143 3.7371 1.3279 3.6739	3386.4 1.5336 2.8263 3.7439 1.3246 3.8173	4423.9 1.6794 2.8522 3.7608 1.3185 4.1216	5682.0 1.8423 2.8807 3.7820 1.3129 4.4508	7119.3 2.0749 2.9121 3.8074 1.3074 4.8073	8811.5 2.2900 2.9467 3.8371 1.3022 5.1936	10804. 2.4608 2.9846 3.8711 1.2969 5.6134	
1400.	P(ATH) 1963.7 Z 1.2779 Cv/R 2.8038 Cp/R 3.8223 Cp/Cv 1.3254 A(KPS) 3.4988	2309.9 1.3331 2.8939 3.8240 1.3216 3.6330	2850.9 1.3913 2.9044 3.8286 1.3186 3.7719	3348.1 1.4526 2.9154 3.8324 1.3146 3.9146	3885.6 1.5172 2.9269 3.8379 1.3112 4.0635	5093.5 1.6574 2.9515 3.8577 1.3050 4.3787	6502.6 1.8136 2.9785 3.8693 1.2991 4.7190	8147.1 1.9882 3.0080 3.8908 1.2935 5.0866	10066. 2.1836 3.0404 3.9160 1.2880 5.4843	12307. 2.4028 3.0760 3.9491 1.2825 5.9149	
1600.	P(ATH) 2231.8 Z 1.2709 Cv/R 2.9096 Cp/R 3.9217 Cp/Cv 1.3135 A(KPS) 3.7057	2713.6 1.3245 2.9953 3.9232 1.3098 3.8435	3233.3 1.3808 3.0095 3.9257 1.3062 3.9863	3793.9 1.4402 3.0160 3.9291 1.3027 4.1345	4398.4 1.5027 3.0271 3.9335 1.2994 4.2861	5753.4 1.6381 3.0507 3.9449 1.2931 4.6128	7320.0 1.7886 3.0764 3.9599 1.2872 4.9627	9161.1 1.9567 3.1044 3.9783 1.2815 5.3399	11290. 2.1433 3.1351 4.0002 1.2760 5.7471	13772. 2.3526 3.1688 4.0254 1.2704 6.1871	
1800.	P(ATH) 2498.4 Z 1.2646 Cv/R 3.0030 Cp/R 4.0155 Cp/Cv 1.3033 A(KPS) 3.8973	3035.1 1.3168 3.0934 4.0183 1.2996 4.0392	3613.1 1.3716 3.1007 4.0288 1.2966 4.1862	4235.7 1.4293 3.1105 4.0287 1.2926 4.3385	4906.1 1.4899 3.1211 4.0242 1.2893 4.4963	6405.2 1.6210 3.1438 4.0338 1.2831 4.8296	8143.1 1.7664 3.1684 4.0466 1.2772 5.1879	10158. 1.9280 3.1953 4.0627 1.2715 5.5736	12494. 2.1080 3.2245 4.0819 1.2659 5.9892	15204. 2.3687 3.2562 4.1042 1.2604 6.4374	
2000.	P(ATH) 2763.7 Z 1.2590 Cv/R 3.1078 Cp/R 4.1011 Cp/Cv 1.2946 A(KPS) 4.0775	3354.6 1.3099 3.1770 4.1014 1.2910 4.2252	3990.3 1.3633 3.1864 4.1074 1.2875 4.3748	4674.0 1.4195 3.1964 4.1045 1.2841 4.5301	5409.3 1.4785 3.2087 4.1073 1.2809 4.6917	7050.1 1.6058 3.2286 4.1154 1.2747 5.0326	8947.0 1.7467 3.2574 4.1260 1.2680 5.3987	11140. 1.9030 3.2782 4.1407 1.2631 5.7920	13676. 2.0766 3.3061 4.1578 1.2576 6.2152	16609. 2.2699 3.3364 4.1777 1.2521 6.6708	
2500.	P(ATH) 3421.9 Z 1.2470 Cv/R 3.3773 Cp/R 4.2790 Cp/Cv 1.2783 A(KPS) 4.4902	4146.4 1.2953 3.3560 4.2787 1.2748 4.6440	4923.9 1.3454 3.3640 4.2783 1.2714 4.8033	5757.5 1.3968 3.3742 4.2791 1.2682 4.9674	6651.3 1.4544 3.3838 4.2807 1.2650 5.1374	8637.3 1.5739 3.4042 4.2860 1.2590 5.4949	10920. 1.7055 3.4262 4.2941 1.2533 5.9776	13544. 1.8500 3.4469 4.3047 1.2478 6.2475	16565. 2.0135 3.4699 4.3178 1.2424 6.7269	20027. 2.1896 3.4949 4.3334 1.2370 7.1984	
3000.	P(ATH) 4074.4 Z 1.2374 Cv/R 3.4845 Cp/R 4.4154 Cp/Cv 1.2672 A(KPS) 4.8020	4930.6 1.2835 3.4927 4.4140 1.2638 4.8228	5846.7 1.3317 3.5012 4.4134 1.2604 5.1888	6826.8 1.3822 3.5100 4.4134 1.2543 5.5372	7875.3 1.4350 3.5191 4.4176 1.2485 5.9188	10196. 1.5483 3.5384 4.4176 1.2429 6.3055	12892. 1.6727 3.5590 4.4235 1.2375 6.7993	15869. 1.8095 3.5811 4.4317 1.2323 7.1823	19364. 2.0180 3.6049 4.4427 1.2263 7.6672	23540. 2.1264 3.6305 4.4548 1.2211 7.6672	

(Table continues)

Table 3 (Continued)

RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GM-MOLE) AND RELATIVE ENTROPY

TEMPERATURE (DEGREE C)	DENSITY (GRAM/GM)																				
	1600. 1650. 1700. 1750. 1800. 1850. 1900. 1950. 2000. 2050.																				
	U-U0	H-H0	(S-S0)/R	U-U0	H-H0	(S-S0)/R	U-U0	H-H0	(S-S0)/R	U-U0	H-H0	(S-S0)/R	U-U0	H-H0	(S-S0)/R	U-U0	H-H0	(S-S0)/R			
500.	1402.7	1492.0	-8.1410	1492.8	1582.9	-8.2938	1583.0	1673.4	-8.4569	1673.4	1764.0	-8.6200	1764.0	1854.8	-8.7832	1854.8	1945.6	-8.9464	1945.6	2036.4	-9.1095
520.	1402.7	1492.0	-8.6072	1492.8	1582.9	-8.1572	1583.0	1673.4	-8.3113	1673.4	1764.0	-8.4654	1764.0	1854.8	-8.6195	1854.8	1945.6	-8.7736	1945.6	2036.4	-8.9367
540.	1373.7	1463.0	-7.8760	1463.0	1553.5	-8.0288	1553.5	1644.0	-8.1819	1644.0	1734.6	-8.3350	1734.6	1825.2	-8.4881	1825.2	1915.8	-8.6412	1915.8	2006.4	-8.7943
560.	1373.7	1463.0	-7.3420	1463.0	1553.5	-7.8920	1553.5	1644.0	-8.0443	1644.0	1734.6	-8.1974	1734.6	1825.2	-8.3515	1825.2	1915.8	-8.5046	1915.8	2006.4	-8.6577
580.	1373.7	1463.0	-6.8080	1463.0	1553.5	-7.3580	1553.5	1644.0	-7.5603	1644.0	1734.6	-7.7154	1734.6	1825.2	-7.8705	1825.2	1915.8	-8.0256	1915.8	2006.4	-8.1728
600.	1343.7	1433.0	-7.2535	1433.0	1523.5	-7.4063	1523.5	1614.0	-7.5594	1614.0	1704.6	-7.7145	1704.6	1795.2	-7.8696	1795.2	1885.8	-8.0247	1885.8	1976.4	-8.1769
620.	1313.7	1403.0	-7.7000	1403.0	1493.5	-7.8528	1493.5	1584.0	-8.0059	1584.0	1674.6	-8.1610	1674.6	1765.2	-8.3161	1765.2	1855.8	-8.4712	1855.8	1946.4	-8.6233
640.	1283.7	1373.0	-7.1465	1373.0	1463.5	-7.2993	1463.5	1554.0	-7.4524	1554.0	1645.2	-7.6075	1645.2	1735.8	-7.7626	1735.8	1826.4	-7.9177	1826.4	1917.0	-8.0728
660.	1253.7	1343.0	-7.5930	1343.0	1433.5	-7.7458	1433.5	1524.0	-7.8989	1524.0	1615.6	-8.0540	1615.6	1706.4	-8.2091	1706.4	1797.0	-8.3592	1797.0	1887.6	-8.5143
680.	1223.7	1313.0	-7.0395	1313.0	1403.5	-7.1923	1403.5	1494.0	-7.3454	1494.0	1586.0	-7.5005	1586.0	1676.6	-7.6556	1676.6	1767.6	-7.8107	1767.6	1858.2	-7.9658
700.	1193.7	1283.0	-6.4860	1283.0	1373.5	-6.6391	1373.5	1464.0	-6.7922	1464.0	1556.6	-6.9473	1556.6	1647.2	-7.1024	1647.2	1737.8	-7.2575	1737.8	1818.4	-7.4126
720.	1163.7	1253.0	-6.9325	1253.0	1343.5	-7.0856	1343.5	1434.0	-7.2381	1434.0	1527.0	-7.3932	1527.0	1617.6	-7.5483	1617.6	1708.6	-7.7034	1708.6	1799.0	-7.8577
740.	1133.7	1223.0	-6.3790	1223.0	1313.5	-6.5321	1313.5	1404.0	-6.6852	1404.0	1497.4	-6.8403	1497.4	1588.4	-7.0004	1588.4	1679.0	-7.1555	1679.0	1779.4	-7.3078
760.	1103.7	1193.0	-5.8255	1193.0	1283.5	-5.9786	1283.5	1374.0	-6.1311	1374.0	1468.6	-6.2862	1468.6	1559.2	-6.4413	1559.2	1649.6	-6.5964	1649.6	1750.0	-6.7029
780.	1073.7	1163.0	-5.2720	1163.0	1253.5	-5.4251	1253.5	1344.0	-5.5802	1344.0	1439.6	-5.7353	1439.6	1530.2	-5.8904	1530.2	1620.6	-6.0455	1620.6	1721.0	-6.2083
800.	1043.7	1133.0	-4.7185	1133.0	1223.5	-4.8716	1223.5	1314.0	-5.0347	1314.0	1410.6	-5.1908	1410.6	1501.2	-5.3459	1501.2	1591.6	-5.5010	1591.6	1692.0	-5.6561
820.	1013.7	1103.0	-4.1650	1103.0	1193.5	-4.3181	1193.5	1284.0	-4.4732	1284.0	1381.6	-4.6283	1381.6	1472.2	-4.7834	1472.2	1562.6	-4.9385	1562.6	1663.0	-5.1112
840.	983.7	1073.0	-3.6115	1073.0	1163.5	-3.7646	1163.5	1254.0	-3.9197	1254.0	1352.6	-4.0748	1352.6	1443.6	-4.2299	1443.6	1533.6	-4.3850	1533.6	1634.0	-4.5391
860.	953.7	1043.0	-3.0580	1043.0	1133.5	-3.2111	1133.5	1224.0	-3.3702	1224.0	1323.6	-3.5253	1323.6	1414.6	-3.6804	1414.6	1504.6	-3.8355	1504.6	1605.0	-4.0002
880.	923.7	1013.0	-2.5045	1013.0	1103.5	-2.6576	1103.5	1194.0	-2.8127	1194.0	1294.6	-2.9678	1294.6	1385.6	-3.1229	1385.6	1475.6	-3.2780	1475.6	1586.0	-3.4321
900.	893.7	983.0	-1.9510	983.0	1073.5	-2.1041	1073.5	1164.0	-2.2592	1164.0	1265.6	-2.4143	1265.6	1356.6	-2.5694	1356.6	1446.6	-2.7245	1446.6	1557.0	-2.8796
920.	863.7	953.0	-1.3975	953.0	1043.5	-1.5516	1043.5	1134.0	-1.7067	1134.0	1236.6	-1.8618	1236.6	1327.6	-2.0169	1327.6	1417.6	-2.1720	1417.6	1528.0	-2.3271
940.	833.7	923.0	-0.8440	923.0	1013.5	-0.9981	1013.5	1104.0	-1.1612	1104.0	1207.6	-1.3173	1207.6	1298.6	-1.4724	1298.6	1388.6	-1.6275	1388.6	1499.0	-1.7826
960.	803.7	893.0	-0.2905	893.0	983.5	-0.4446	983.5	1074.0	-0.6167	1074.0	1178.6	-1.0228	1178.6	1269.6	-1.1779	1269.6	1359.6	-1.3330	1359.6	1460.0	-1.4877
980.	773.7	863.0	0.2630	863.0	953.5	0.1089	953.5	1044.0	0.2740	1044.0	1149.6	-0.7779	1149.6	1240.6	-0.9280	1240.6	1330.6	-1.0881	1330.6	1441.0	-1.2428
1000.	743.7	833.0	0.7145	833.0	923.5	0.5604	923.5	1014.0	0.7295	1014.0	1120.6	-0.6280	1120.6	1211.6	-0.8831	1211.6	1301.6	-1.1382	1301.6	1422.0	-1.3929

(Table continues)

Table 3 (Continued)

		RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GM-MOLE) AND RELATIVE ENTROPY									
TEMPERATURE (DEGREES K)		UNITS(ATMOSPHERE)									
		1600.	1650.	1700.	1750.	1800.	1850.	1900.	1950.	2000.	2060.
1020.	U-U0	4868.6	4976.5	5068.6	5155.7	5227.4	5287.4	5331.0	5365.8	5391.5	5409.5
	H-H0	14212.	14289.	14358.	14431.	14500.	14565.	14627.	14686.	14742.	14796.
	(S-S0)/R	-5.7731	-5.8052	-5.8367	-5.8673	-5.8970	-5.9258	-5.9538	-5.9811	-5.9974	-6.0132

(Table continues)

Table 3 (Continued)

RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GM-MOLE) AND RELATIVE ENTROPY

TEMPERATURE (DEGREES K)	DENSITY (GRAMS/GM-MOLE)									
	1600.	1650.	1700.	1750.	1800.	1850.	1900.	1950.	2000.	2000.
1540. U-U0	8343.6	6466.6	6590.6	6739.7	6891.7	6952.5	6229.8	6411.8	6611.5	
H-H0	21072.	21934.	22656.	23440.	24094.	24623.	27233.	28330.	29924.	
(S-S0)/R	-4.1974	-4.4963	-4.5917	-4.6877	-4.7885	-4.8801	-4.9860	-5.0899	-5.1922	

(Table continues)

Table 3 (Continued)

RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GM-MOLE) AND RELATIVE ENTROPY

TEMPERATURE (°C/MOL)	DENSITY (GRAMS/CM ³)									
	1600.	1650.	1700.	1750.	1800.	1850.	1900.	1950.	2000.	
2000.	U-U0	11976.	12177.	12296.	12423.	12547.	12664.	12774.	12877.	12974.
	H-H0	27747.	28746.	29000.	29400.	29744.	30144.	30597.	31050.	31514.
	(S-S0)/R	-3.3761	-3.4849	-3.5932	-3.6922	-3.7915	-3.8912	-3.9914	-4.0921	-4.1932
2050.	U-U0	12117.	12271.	12439.	12609.	12785.	12963.	13144.	13329.	13519.
	H-H0	28602.	29604.	29874.	30374.	30874.	31374.	31874.	32374.	32874.
	(S-S0)/R	-3.3412	-3.4299	-3.5179	-3.6059	-3.6939	-3.7819	-3.8699	-3.9579	-4.0459
2100.	U-U0	12261.	12436.	12621.	12814.	13014.	13214.	13414.	13614.	13814.
	H-H0	29458.	29746.	29874.	30174.	30474.	30774.	31074.	31374.	31674.
	(S-S0)/R	-3.3167	-3.3849	-3.4529	-3.5209	-3.5889	-3.6569	-3.7249	-3.7929	-3.8609
2150.	U-U0	12404.	12599.	12804.	13014.	13224.	13434.	13644.	13854.	14064.
	H-H0	29923.	29974.	30024.	30174.	30324.	30474.	30624.	30774.	30924.
	(S-S0)/R	-3.2725	-3.3202	-3.3679	-3.4156	-3.4633	-3.5110	-3.5587	-3.6064	-3.6541
2200.	U-U0	12548.	12759.	12974.	13194.	13414.	13634.	13854.	14074.	14294.
	H-H0	29974.	29746.	29518.	29290.	29062.	28834.	28606.	28378.	28150.
	(S-S0)/R	-3.2389	-3.2799	-3.3209	-3.3619	-3.4029	-3.4439	-3.4849	-3.5259	-3.5669
2250.	U-U0	12692.	12924.	13164.	13404.	13644.	13884.	14124.	14364.	14604.
	H-H0	29924.	29746.	29568.	29390.	29212.	29034.	28856.	28678.	28500.
	(S-S0)/R	-3.2053	-3.2362	-3.2671	-3.2980	-3.3289	-3.3598	-3.3907	-3.4216	-3.4525
2300.	U-U0	12837.	13074.	13314.	13554.	13794.	14034.	14274.	14514.	14754.
	H-H0	29774.	29596.	29418.	29240.	29062.	28884.	28706.	28528.	28350.
	(S-S0)/R	-3.1717	-3.1926	-3.2135	-3.2344	-3.2553	-3.2762	-3.2971	-3.3180	-3.3389
2350.	U-U0	12981.	13224.	13464.	13704.	13944.	14184.	14424.	14664.	14904.
	H-H0	29524.	29346.	29168.	28990.	28812.	28634.	28456.	28278.	28100.
	(S-S0)/R	-3.1381	-3.1490	-3.1599	-3.1708	-3.1817	-3.1926	-3.2035	-3.2144	-3.2253
2400.	U-U0	13126.	13374.	13614.	13854.	14094.	14334.	14574.	14814.	15054.
	H-H0	29274.	29096.	28918.	28740.	28562.	28384.	28206.	28028.	27850.
	(S-S0)/R	-3.1045	-3.1054	-3.1063	-3.1072	-3.1081	-3.1090	-3.1099	-3.1108	-3.1117
2450.	U-U0	13271.	13524.	13764.	14004.	14244.	14484.	14724.	14964.	15204.
	H-H0	29024.	28846.	28668.	28490.	28312.	28134.	27956.	27778.	27600.
	(S-S0)/R	-3.0709	-3.0618	-3.0527	-3.0436	-3.0345	-3.0254	-3.0163	-3.0072	-2.9981
2500.	U-U0	13416.	13674.	13914.	14154.	14394.	14634.	14874.	15114.	15354.
	H-H0	28774.	28596.	28418.	28240.	28062.	27884.	27706.	27528.	27350.
	(S-S0)/R	-3.0373	-3.0282	-3.0191	-3.0100	-3.0009	-2.9918	-2.9827	-2.9736	-2.9645
2550.	U-U0	13561.	13824.	14064.	14304.	14544.	14784.	15024.	15264.	15504.
	H-H0	28524.	28346.	28168.	27990.	27812.	27634.	27456.	27278.	27100.
	(S-S0)/R	-2.9937	-2.9846	-2.9755	-2.9664	-2.9573	-2.9482	-2.9391	-2.9300	-2.9209
2600.	U-U0	13706.	13974.	14214.	14454.	14694.	14934.	15174.	15414.	15654.
	H-H0	28274.	28096.	27918.	27740.	27562.	27384.	27206.	27028.	26850.
	(S-S0)/R	-2.9601	-2.9510	-2.9419	-2.9328	-2.9237	-2.9146	-2.9055	-2.8964	-2.8873
2650.	U-U0	13851.	14124.	14364.	14604.	14844.	15084.	15324.	15564.	15804.
	H-H0	28024.	27846.	27668.	27490.	27312.	27134.	26956.	26778.	26600.
	(S-S0)/R	-2.9265	-2.9174	-2.9083	-2.8992	-2.8901	-2.8810	-2.8719	-2.8628	-2.8537
2700.	U-U0	13996.	14274.	14514.	14754.	14994.	15234.	15474.	15714.	15954.
	H-H0	27774.	27596.	27418.	27240.	27062.	26884.	26706.	26528.	26350.
	(S-S0)/R	-2.8929	-2.8838	-2.8747	-2.8656	-2.8565	-2.8474	-2.8383	-2.8292	-2.8201
2750.	U-U0	14141.	14424.	14664.	14904.	15144.	15384.	15624.	15864.	16104.
	H-H0	27524.	27346.	27168.	26990.	26812.	26634.	26456.	26278.	26100.
	(S-S0)/R	-2.8593	-2.8502	-2.8411	-2.8320	-2.8229	-2.8138	-2.8047	-2.7956	-2.7865
2800.	U-U0	14286.	14574.	14814.	15054.	15294.	15534.	15774.	16014.	16254.
	H-H0	27274.	27096.	26918.	26740.	26562.	26384.	26206.	26028.	25850.
	(S-S0)/R	-2.8257	-2.8166	-2.8075	-2.7984	-2.7893	-2.7802	-2.7711	-2.7620	-2.7529
2850.	U-U0	14431.	14724.	14964.	15204.	15444.	15684.	15924.	16164.	16404.
	H-H0	27024.	26846.	26668.	26490.	26312.	26134.	25956.	25778.	25600.
	(S-S0)/R	-2.7921	-2.7830	-2.7739	-2.7648	-2.7557	-2.7466	-2.7375	-2.7284	-2.7193
2900.	U-U0	14576.	14874.	15114.	15354.	15594.	15834.	16074.	16314.	16554.
	H-H0	26774.	26596.	26418.	26240.	26062.	25884.	25706.	25528.	25350.
	(S-S0)/R	-2.7585	-2.7494	-2.7403	-2.7312	-2.7221	-2.7130	-2.7039	-2.6948	-2.6857
2950.	U-U0	14721.	15024.	15264.	15504.	15744.	15984.	16224.	16464.	16704.
	H-H0	26524.	26346.	26168.	25990.	25812.	25634.	25456.	25278.	25100.
	(S-S0)/R	-2.7249	-2.7158	-2.7067	-2.6976	-2.6885	-2.6794	-2.6703	-2.6612	-2.6521
3000.	U-U0	14866.	15174.	15414.	15654.	15894.	16134.	16374.	16614.	16854.
	H-H0	26274.	26096.	25918.	25740.	25562.	25384.	25206.	25028.	24850.
	(S-S0)/R	-2.6913	-2.6822	-2.6731	-2.6640	-2.6549	-2.6458	-2.6367	-2.6276	-2.6185

(Table continues)

Table 3 (Continued)

RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GRAM-MOLE) AND RELATIVE ENTROPY

TEMPERATURE (DEGREE C)	DENSITY (GRAMS/CM ³)											
	1	10	50	100	150	200	250	300	350	400	450	
2500	U-U0 H-H0 (S-S0)/R	11111 17607 0.0771	11117 17716 0.0773	11116 17710 0.0773	11103 17617 1.4138	11222 18190 0.9782	11262 18644 0.8599	11344 18918 0.6955	11349 18918 0.5916	11395 19000 0.0090	11444 19168 -0.1615	11495 19286 -0.5127
2600	U-U0 H-H0 (S-S0)/R	11243 17808 0.1020	11240 17928 0.1023	11278 18068 2.1823	11316 18222 1.4398	11355 18388 1.0141	11395 18568 0.8450	11478 18758 0.4415	11483 18758 0.2175	11538 18668 0.0321	11594 18978 -0.1193	11655 19288 -0.7885
2620	U-U0 H-H0 (S-S0)/R	11374 18041 0.1200	11382 18081 0.1204	11411 18087 2.1878	11448 18097 1.0253	11488 18097 1.0222	11529 18088 0.7114	11572 18078 0.4427	11587 18078 0.2436	11644 18068 0.0577	11704 18058 -0.1192	11768 18048 -0.7290
2640	U-U0 H-H0 (S-S0)/R	11509 18278 0.1356	11515 18294 0.1362	11544 18288 2.1134	11582 18288 1.4398	11622 18288 0.8594	11663 18278 0.7322	11706 18268 0.4436	11722 18268 0.2492	11789 18258 0.0629	11849 18248 -0.0833	11911 18238 -0.7344
2660	U-U0 H-H0 (S-S0)/R	11642 18488 0.1498	11648 18527 0.1503	11678 18510 2.1487	11716 18498 1.5182	11755 18488 1.0388	11797 18478 0.7427	11841 18468 0.5288	11856 18468 0.2948	11924 18458 0.1086	11984 18448 -0.0776	12047 18438 -0.7288
2680	U-U0 H-H0 (S-S0)/R	11775 18698 0.1624	11781 18737 0.1629	11811 18720 2.1781	11848 18708 1.5434	11888 18698 1.0641	11931 18688 0.7680	11975 18678 0.5346	11990 18678 0.3202	12058 18668 0.1341	12118 18658 -0.0470	12181 18648 -0.7280
2700	U-U0 H-H0 (S-S0)/R	11908 18908 0.1741	11914 18947 0.1746	11944 18930 2.2079	11982 18918 1.5680	12022 18908 1.0888	12065 18898 0.7927	12109 18888 0.5406	12124 18888 0.3262	12192 18878 0.1401	12252 18868 -0.0470	12315 18858 -0.7280
2720	U-U0 H-H0 (S-S0)/R	12042 19118 0.1856	12048 19157 0.1861	12078 19140 2.2373	12116 19128 1.5924	12155 19118 1.1088	12199 19108 0.8127	12243 19098 0.5406	12258 19098 0.3262	12326 19088 0.1401	12386 19078 -0.0470	12449 19068 -0.7280
2740	U-U0 H-H0 (S-S0)/R	12176 19328 0.1971	12182 19367 0.1976	12212 19350 2.2667	12250 19338 1.6162	12290 19328 1.1288	12333 19318 0.8227	12377 19308 0.5406	12392 19308 0.3262	12460 19298 0.1401	12520 19288 -0.0470	12583 19278 -0.7280
2760	U-U0 H-H0 (S-S0)/R	12310 19538 0.2086	12316 19577 0.2091	12346 19560 2.2961	12384 19548 1.6302	12424 19538 1.1418	12467 19528 0.8357	12511 19518 0.5406	12526 19518 0.3262	12594 19508 0.1401	12654 19498 -0.0470	12717 19488 -0.7280
2780	U-U0 H-H0 (S-S0)/R	12444 19748 0.2201	12450 19787 0.2206	12480 19770 2.3255	12518 19758 1.6422	12558 19748 1.1538	12601 19738 0.8487	12645 19728 0.5406	12660 19728 0.3262	12728 19718 0.1401	12788 19708 -0.0470	12851 19698 -0.7280
2800	U-U0 H-H0 (S-S0)/R	12578 19958 0.2316	12584 19997 0.2321	12614 19980 2.3549	12652 19968 1.6536	12692 19958 1.1652	12735 19948 0.8501	12779 19938 0.5406	12794 19938 0.3262	12862 19928 0.1401	12922 19918 -0.0470	12985 19908 -0.7280
2820	U-U0 H-H0 (S-S0)/R	12712 20168 0.2431	12718 20207 0.2436	12748 20190 2.3843	12786 20178 1.6642	12826 20168 1.1768	12869 20158 0.8517	12913 20148 0.5406	12928 20148 0.3262	12996 20138 0.1401	13056 20128 -0.0470	13119 20118 -0.7280
2840	U-U0 H-H0 (S-S0)/R	12846 20378 0.2546	12852 20417 0.2551	12882 20400 2.4137	12920 20388 1.6752	12960 20378 1.1884	12993 20368 0.8522	13037 20358 0.5406	13052 20358 0.3262	13120 20348 0.1401	13180 20338 -0.0470	13243 20328 -0.7280
2860	U-U0 H-H0 (S-S0)/R	12980 20588 0.2661	12986 20627 0.2666	13016 20610 2.4431	13054 20598 1.6856	13094 20588 1.2000	13137 20578 0.8531	13181 20568 0.5406	13196 20568 0.3262	13264 20558 0.1401	13324 20548 -0.0470	13387 20538 -0.7280
2880	U-U0 H-H0 (S-S0)/R	13114 20798 0.2776	13120 20837 0.2781	13150 20820 2.4725	13188 20808 1.6950	13228 20798 1.2114	13271 20788 0.8556	13315 20778 0.5406	13330 20778 0.3262	13398 20768 0.1401	13458 20758 -0.0470	13521 20748 -0.7280
2900	U-U0 H-H0 (S-S0)/R	13248 21008 0.2891	13254 21047 0.2896	13284 21030 2.5019	13322 21018 1.7044	13362 21008 1.2228	13405 20998 0.8581	13449 20988 0.5406	13464 20988 0.3262	13532 20978 0.1401	13592 20968 -0.0470	13655 20958 -0.7280
2920	U-U0 H-H0 (S-S0)/R	13382 21218 0.3006	13388 21257 0.3011	13418 21240 2.5313	13456 21228 1.7138	13496 21218 1.2342	13539 21208 0.8607	13583 21198 0.5406	13598 21198 0.3262	13666 21188 0.1401	13726 21178 -0.0470	13789 21168 -0.7280
2940	U-U0 H-H0 (S-S0)/R	13516 21428 0.3121	13522 21467 0.3126	13552 21450 2.5607	13590 21438 1.7242	13630 21428 1.2456	13673 21418 0.8632	13717 21408 0.5406	13732 21408 0.3262	13800 21398 0.1401	13860 21388 -0.0470	13923 21378 -0.7280
2960	U-U0 H-H0 (S-S0)/R	13650 21638 0.3236	13656 21677 0.3241	13686 21660 2.5901	13724 21648 1.7346	13764 21638 1.2570	13807 21628 0.8657	13851 21618 0.5406	13866 21618 0.3262	13934 21608 0.1401	14004 21598 -0.0470	14067 21588 -0.7280
2980	U-U0 H-H0 (S-S0)/R	13784 21848 0.3351	13790 21887 0.3356	13820 21870 2.6195	13858 21858 1.7450	13898 21848 1.2684	13941 21838 0.8683	13985 21828 0.5406	14000 21828 0.3262	14068 21818 0.1401	14128 21808 -0.0470	14191 21798 -0.7280
3000	U-U0 H-H0 (S-S0)/R	13918 22058 0.3466	13924 22097 0.3471	13954 22080 2.6489	13992 22068 1.7544	14032 22058 1.2798	14075 22048 0.8709	14119 22038 0.5406	14134 22038 0.3262	14202 22028 0.1401	14262 22018 -0.0470	14325 22008 -0.7280

(Table continues)

Table 3 (Continued)

TEMPERATURE (DEGREE C)	RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GM-MOLE) AND RELATIVE ENTROPY											
	DENSITY (MAGAT)											
	500.	520.	600.	650.	700.	750.	800.	850.	900.	950.	1000.	
2580.	U-U0 H-H0 (S-S0)/R	13549. 26442. -0.4522	15005. 26794. -0.5022	15004. 27104. -0.7046	15725. 27592. -0.8266	15790. 27858. -0.9214	15854. 28106. -1.0378	15930. 28376. -1.1404	16005. 28670. -1.2359	16084. 28985. -1.3264	16168. 29307. -1.4227	16259. 29637. -1.5230
2600.	U-U0 H-H0 (S-S0)/R	13604. 26631. -0.4250	15741. 26985. -0.5558	13600. 27157. -0.6781	13862. 27447. -0.7941	13927. 27556. -0.9048	13996. 27706. -1.0110	14068. 27886. -1.1135	14144. 28094. -1.2128	14223. 28322. -1.3094	14307. 28567. -1.4038	14395. 28909. -1.4958
2620.	U-U0 H-H0 (S-S0)/R	13622. 26820. -0.3997	13877. 27176. -0.5295	13934. 27350. -0.6518	13989. 27542. -0.7676	14055. 27766. -0.8763	14134. 28026. -0.9844	14206. 28316. -1.0868	14283. 28638. -1.1825	14363. 28994. -1.2725	14447. 29386. -1.3560	14536. 29814. -1.4407
2640.	U-U0 H-H0 (S-S0)/R	13956. 27009. -0.3736	14013. 27167. -0.5034	14073. 27341. -0.6256	14136. 27531. -0.7414	14202. 27748. -0.8510	14272. 27996. -0.9580	14345. 28278. -1.0603	14422. 28598. -1.1590	14502. 28957. -1.2550	14587. 29356. -1.3488	14676. 29806. -1.4418
2660.	U-U0 H-H0 (S-S0)/R	14092. 27199. -0.3478	14150. 27359. -0.4775	14210. 27537. -0.5986	14274. 27734. -0.7153	14340. 27952. -0.8257	14410. 28204. -0.9317	14484. 28484. -1.0340	14562. 28796. -1.1320	14642. 29234. -1.2262	14727. 29721. -1.3178	14817. 30259. -1.4150
2680.	U-U0 H-H0 (S-S0)/R	14228. 27388. -0.3220	14286. 27551. -0.4517	14347. 27731. -0.5707	14411. 27946. -0.6893	14478. 28194. -0.7997	14549. 28478. -0.9056	14623. 28798. -1.0078	14700. 29138. -1.1067	14782. 29538. -1.2029	14868. 29991. -1.2967	14959. 30572. -1.3884
2700.	U-U0 H-H0 (S-S0)/R	14365. 27578. -0.2965	14423. 27743. -0.4261	14485. 27938. -0.5450	14549. 28164. -0.6635	14627. 28424. -0.7739	14702. 28720. -0.8797	14780. 29056. -0.9817	14860. 29438. -1.0805	14922. 29871. -1.1766	14999. 30369. -1.2713	15100. 30936. -1.3620
2720.	U-U0 H-H0 (S-S0)/R	14502. 27768. -0.2711	14561. 27935. -0.4008	14622. 28130. -0.5204	14687. 28354. -0.6379	14755. 28608. -0.7461	14826. 28894. -0.8538	14901. 29224. -0.9558	14980. 29596. -1.0546	15063. 29991. -1.1505	15150. 30521. -1.2441	15241. 31099. -1.3357
2740.	U-U0 H-H0 (S-S0)/R	14639. 27959. -0.2458	14698. 28127. -0.3754	14760. 28333. -0.4970	14825. 28576. -0.6174	14894. 28848. -0.7225	14966. 29152. -0.8202	15041. 29496. -0.9201	15120. 29884. -1.0207	15203. 30319. -1.1240	15291. 30801. -1.2281	15383. 31359. -1.3308
2760.	U-U0 H-H0 (S-S0)/R	14776. 28149. -0.2206	14836. 28319. -0.3500	14898. 28528. -0.4717	14964. 28768. -0.5870	15033. 29042. -0.6973	15105. 29354. -0.8027	15181. 29696. -0.9045	15260. 30088. -1.0030	15344. 30521. -1.0980	15432. 31006. -1.1983	15525. 31529. -1.2956
2780.	U-U0 H-H0 (S-S0)/R	14914. 28340. -0.1957	14974. 28517. -0.3250	15037. 28722. -0.4466	15103. 28968. -0.5610	15172. 29248. -0.6718	15245. 29572. -0.7773	15321. 29944. -0.8790	15400. 30368. -0.9775	15483. 30844. -1.0782	15570. 31391. -1.1809	15667. 31972. -1.2858
2800.	U-U0 H-H0 (S-S0)/R	15051. 28531. -0.1708	15112. 28708. -0.3000	15175. 28922. -0.4216	15242. 29176. -0.5368	15311. 29464. -0.6467	15384. 29798. -0.7521	15461. 30168. -0.8537	15542. 30588. -0.9521	15626. 31061. -1.0477	15715. 31599. -1.1443	15809. 32169. -1.2321
2820.	U-U0 H-H0 (S-S0)/R	15189. 28721. -0.1461	15250. 28908. -0.2751	15314. 29142. -0.3967	15381. 29426. -0.5118	15451. 29744. -0.6217	15524. 30108. -0.7270	15601. 30518. -0.8285	15683. 30988. -0.9269	15768. 31521. -1.0224	15857. 32109. -1.1159	15951. 32748. -1.2086
2840.	U-U0 H-H0 (S-S0)/R	15327. 28913. -0.1219	15389. 29101. -0.2506	15453. 29347. -0.3720	15520. 29643. -0.4871	15590. 29992. -0.5968	15664. 30358. -0.7021	15742. 30754. -0.8035	15824. 31196. -0.9018	15909. 31681. -0.9972	15999. 32229. -1.0903	16 04. 32817. -1.1817
2860.	U-U0 H-H0 (S-S0)/R	15466. 29104. -0.0971	15527. 29294. -0.2261	15592. 29542. -0.3474	15660. 29849. -0.4624	15730. 30218. -0.5721	15805. 30564. -0.6773	15883. 30928. -0.7787	15965. 31331. -0.8768	16051. 31788. -0.9722	16142. 32294. -1.0651	16237. 32867. -1.1560
2880.	U-U0 H-H0 (S-S0)/R	15604. 29295. -0.0728	15666. 29488. -0.2017	15731. 29748. -0.3230	15799. 30066. -0.4379	15871. 30448. -0.5475	15945. 30888. -0.6528	16024. 31391. -0.7539	16106. 31951. -0.8520	16193. 32521. -0.9472	16284. 33109. -1.0401	16380. 33689. -1.1309
2900.	U-U0 H-H0 (S-S0)/R	15743. 29487. -0.0486	15805. 29681. -0.1775	15871. 29947. -0.2987	15939. 30278. -0.4135	16011. 30678. -0.5230	16086. 31141. -0.6281	16165. 31671. -0.7293	16248. 32258. -0.8273	16335. 32887. -0.9225	16427. 33543. -1.0153	16521. 34229. -1.1080
2920.	U-U0 H-H0 (S-S0)/R	15882. 29678. -0.0246	15945. 29874. -0.1534	16010. 30148. -0.2745	16079. 30484. -0.3893	16151. 30884. -0.4987	16227. 31348. -0.6037	16307. 31831. -0.7048	16390. 32338. -0.8027	16478. 32864. -0.8978	16570. 33439. -0.9919	16666. 34047. -1.0812
2940.	U-U0 H-H0 (S-S0)/R	16021. 29869. -0.0007	16084. 30072. -0.1294	16150. 30402. -0.2505	16220. 30752. -0.3652	16292. 31128. -0.4746	16368. 31536. -0.5794	16448. 31984. -0.6805	16532. 32468. -0.7785	16620. 32991. -0.8733	16711. 33529. -0.9640	16806. 34169. -1.0526
2960.	U-U0 H-H0 (S-S0)/R	16160. 30061. 0.0231	16224. 30281. -0.1056	16290. 30636. -0.2266	16360. 31022. -0.3412	16433. 31436. -0.4505	16510. 31884. -0.5553	16590. 32381. -0.6560	16674. 32928. -0.7540	16763. 33481. -0.8490	16856. 34049. -0.9440	16954. 34641. -1.0323
2980.	U-U0 H-H0 (S-S0)/R	16300. 30254. 0.0467	16364. 30491. -0.2019	16431. 30858. -0.3228	16501. 31252. -0.4374	16574. 31682. -0.5488	16651. 32144. -0.6513	16732. 32636. -0.7557	16817. 33158. -0.8500	16906. 33691. -0.9440	16999. 34269. -1.0340	17096. 34841. -1.1220
3000.	U-U0 H-H0 (S-S0)/R	16440. 30448. 0.0703	16504. 30731. -0.2819	16571. 31136. -0.4028	16641. 31562. -0.5182	16714. 32018. -0.6288	16791. 32494. -0.7353	16872. 32991. -0.8387	16957. 33508. -0.9380	17046. 34049. -1.0340	17139. 34619. -1.1280	17237. 35211. -1.2200

(Table continues)

Table 3 (Continued)

RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GM-MOLE) AND RELATIVE ENTROPY

TEMPERATURE (DEGREE K)	DENSITY (GRAMS/L)										
	1090.	1100.	1120.	1150.	1180.	1200.	1250.	1300.	1400.	1500.	
2580	U-U0 14147 -1.0150	U-H0 14445 -1.7027	U-H0 14547 -1.7865	U-H0 14655 -1.8775	U-H0 14769 -1.9651	U-H0 14889 -2.0485	U-H0 15016 -2.1279	U-H0 15150 -2.2038	U-H0 15291 -2.2764	U-H0 15439 -2.3460	U-H0 15594 -2.4127
2600	U-U0 14408 -1.5867	U-H0 14686 -2.2684	U-H0 14809 -2.3429	U-H0 14938 -2.4196	U-H0 15072 -2.4985	U-H0 15211 -2.5797	U-H0 15355 -2.6633	U-H0 15504 -2.7495	U-H0 15658 -2.8277	U-H0 15817 -2.9084	U-H0 15981 -2.9917
2620	U-U0 14669 -1.5520	U-H0 14928 -2.2403	U-H0 15031 -2.3159	U-H0 15140 -2.3937	U-H0 15254 -2.4738	U-H0 15373 -2.5562	U-H0 15497 -2.6410	U-H0 15626 -2.7273	U-H0 15760 -2.8111	U-H0 15899 -2.8974	U-H0 16043 -2.9862
2640	U-U0 14770 -1.5320	U-H0 14989 -2.2222	U-H0 15074 -2.2987	U-H0 15165 -2.3776	U-H0 15261 -2.4590	U-H0 15362 -2.5420	U-H0 15468 -2.6276	U-H0 15579 -2.7059	U-H0 15694 -2.7880	U-H0 15814 -2.8729	U-H0 15939 -2.9597
2660	U-U0 14913 -1.5057	U-H0 15011 -2.1958	U-H0 15086 -2.2725	U-H0 15167 -2.3519	U-H0 15253 -2.4340	U-H0 15345 -2.5189	U-H0 15442 -2.6067	U-H0 15544 -2.6974	U-H0 15651 -2.7911	U-H0 15763 -2.8878	U-H0 15880 -2.9876
2680	U-U0 15053 -1.4785	U-H0 15155 -2.1673	U-H0 15229 -2.2452	U-H0 15308 -2.3261	U-H0 15392 -2.4100	U-H0 15481 -2.4970	U-H0 15575 -2.5871	U-H0 15674 -2.6894	U-H0 15778 -2.7849	U-H0 15887 -2.8836	U-H0 15999 -2.9857
2700	U-U0 15195 -1.4499	U-H0 15296 -2.1359	U-H0 15370 -2.2147	U-H0 15449 -2.2966	U-H0 15533 -2.3816	U-H0 15622 -2.4700	U-H0 15716 -2.5619	U-H0 15814 -2.6564	U-H0 15917 -2.7557	U-H0 16024 -2.8580	U-H0 16136 -2.9623
2720	U-U0 15337 -1.4255	U-H0 15436 -2.1049	U-H0 15509 -2.1847	U-H0 15587 -2.2678	U-H0 15670 -2.3540	U-H0 15758 -2.4435	U-H0 15851 -2.5364	U-H0 15948 -2.6330	U-H0 16050 -2.7273	U-H0 16157 -2.8264	U-H0 16269 -2.9323
2740	U-U0 15479 -1.3993	U-H0 15581 -2.0744	U-H0 15654 -2.1553	U-H0 15731 -2.2394	U-H0 15813 -2.3267	U-H0 15900 -2.4173	U-H0 15992 -2.5114	U-H0 16088 -2.6091	U-H0 16189 -2.7096	U-H0 16294 -2.8120	U-H0 16404 -2.9174
2760	U-U0 15622 -1.3737	U-H0 15724 -2.0453	U-H0 15797 -2.1272	U-H0 15874 -2.2123	U-H0 15955 -2.3009	U-H0 16040 -2.3832	U-H0 16129 -2.4692	U-H0 16222 -2.5579	U-H0 16319 -2.6503	U-H0 16420 -2.7377	U-H0 16525 -2.8281
2780	U-U0 15764 -1.3473	U-H0 15827 -2.0172	U-H0 15900 -2.1001	U-H0 15977 -2.1857	U-H0 16058 -2.2740	U-H0 16143 -2.3660	U-H0 16232 -2.4617	U-H0 16324 -2.5513	U-H0 16420 -2.6438	U-H0 16520 -2.7325	U-H0 16624 -2.8218
2800	U-U0 15907 -1.3215	U-H0 15971 -1.9904	U-H0 16044 -2.0742	U-H0 16121 -2.1607	U-H0 16202 -2.2500	U-H0 16286 -2.3423	U-H0 16374 -2.4376	U-H0 16466 -2.5360	U-H0 16561 -2.6284	U-H0 16660 -2.7268	U-H0 16763 -2.8229
2820	U-U0 16050 -1.2959	U-H0 16124 -1.9702	U-H0 16207 -2.0549	U-H0 16294 -2.1423	U-H0 16385 -2.2337	U-H0 16480 -2.3283	U-H0 16578 -2.4272	U-H0 16680 -2.5295	U-H0 16785 -2.6322	U-H0 16894 -2.7400	U-H0 17007 -2.8474
2840	U-U0 16193 -1.2705	U-H0 16268 -1.9445	U-H0 16351 -2.0392	U-H0 16438 -2.1367	U-H0 16529 -2.2371	U-H0 16624 -2.3406	U-H0 16722 -2.4472	U-H0 16824 -2.5570	U-H0 16929 -2.6761	U-H0 17038 -2.8073	U-H0 17150 -2.9297
2860	U-U0 16337 -1.2451	U-H0 16412 -1.9197	U-H0 16495 -2.0352	U-H0 16582 -2.1437	U-H0 16673 -2.2552	U-H0 16767 -2.3698	U-H0 16864 -2.4886	U-H0 16964 -2.6216	U-H0 17067 -2.7575	U-H0 17174 -2.8923	U-H0 17285 -3.0197
2880	U-U0 16480 -1.2207	U-H0 16488 -1.8953	U-H0 16571 -2.0108	U-H0 16658 -2.1193	U-H0 16749 -2.2318	U-H0 16843 -2.3474	U-H0 16940 -2.4662	U-H0 17040 -2.6081	U-H0 17143 -2.7531	U-H0 17250 -2.9040	U-H0 17361 -3.0789
2900	U-U0 16624 -1.1949	U-H0 16631 -1.8709	U-H0 16714 -1.9864	U-H0 16801 -2.0949	U-H0 16892 -2.2164	U-H0 16986 -2.3410	U-H0 17083 -2.4788	U-H0 17183 -2.6207	U-H0 17286 -2.7735	U-H0 17393 -2.9283	U-H0 17504 -3.1532
2920	U-U0 16768 -1.1700	U-H0 16775 -1.8465	U-H0 16858 -1.9620	U-H0 16945 -2.0705	U-H0 17036 -2.1920	U-H0 17130 -2.3266	U-H0 17227 -2.4744	U-H0 17327 -2.6162	U-H0 17430 -2.7800	U-H0 17537 -2.9577	U-H0 17648 -3.2279
2940	U-U0 16912 -1.1457	U-H0 16920 -1.8224	U-H0 17003 -1.9379	U-H0 17090 -2.0504	U-H0 17181 -2.1719	U-H0 17275 -2.3065	U-H0 17372 -2.4543	U-H0 17472 -2.6061	U-H0 17575 -2.7719	U-H0 17682 -2.9436	U-H0 17794 -3.2817
2960	U-U0 17057 -1.1200	U-H0 17065 -1.7977	U-H0 17148 -1.9132	U-H0 17235 -2.0257	U-H0 17326 -2.1472	U-H0 17420 -2.2818	U-H0 17517 -2.4296	U-H0 17617 -2.5914	U-H0 17720 -2.7672	U-H0 17827 -2.9570	U-H0 17939 -3.2364
2980	U-U0 17201 -1.0941	U-H0 17210 -1.7734	U-H0 17293 -1.8889	U-H0 17380 -2.0014	U-H0 17471 -2.1229	U-H0 17565 -2.2575	U-H0 17662 -2.4153	U-H0 17762 -2.5771	U-H0 17865 -2.7629	U-H0 17972 -2.9287	U-H0 18084 -3.2011
3000	U-U0 17346 -1.0716	U-H0 17355 -1.7531	U-H0 17438 -1.8686	U-H0 17525 -1.9911	U-H0 17616 -2.1126	U-H0 17710 -2.2472	U-H0 17807 -2.4000	U-H0 17907 -2.5618	U-H0 18010 -2.7376	U-H0 18117 -2.9233	U-H0 18229 -3.1754

(Table continues)

Table 3 (Continued)

TEMPERATURE (DEGREE K)	RELATIVE INTERNAL ENERGY AND ENTHALPY (CALORIES/GM-MOLE) AND RELATIVE ENTROPY									
						DENSITY (AMAGAT)				
	1000.	1000.	1700.	1700.	1000.	1000.	1000.	1000.	1000.	1000.
2500. U-U0	19767.	19769.	16134.	16135.	16545.	16710.	17010.	17244.	17335.	17335.
H-H0	34366.	34463.	30440.	30441.	37019.	39249.	40862.	42144.	43740.	45459.
(S-S0)/R	-2.5561	-2.6331	-2.7162	-2.7593	-2.8026	-2.8461	-2.8903	-2.9350	-2.9803	-3.0260
2600. U-U0	19916.	19919.	16284.	16285.	16695.	16860.	17160.	17394.	17485.	17485.
H-H0	34620.	34717.	30694.	30695.	37273.	39503.	41116.	42398.	43994.	45713.
(S-S0)/R	-2.5212	-2.6000	-2.6849	-2.7299	-2.7730	-2.8163	-2.8605	-2.9052	-2.9503	-2.9959
2620. U-U0	19969.	19972.	16337.	16338.	16748.	16913.	17213.	17447.	17538.	17538.
H-H0	34874.	34971.	30848.	30849.	37427.	39657.	41270.	42552.	44148.	45867.
(S-S0)/R	-2.4999	-2.5792	-2.6649	-2.7100	-2.7531	-2.7964	-2.8406	-2.8853	-2.9303	-2.9759
2640. U-U0	16216.	16219.	16599.	16600.	16980.	17145.	17310.	17475.	17566.	17566.
H-H0	35131.	35228.	31214.	31215.	37793.	40023.	41636.	42918.	44514.	46233.
(S-S0)/R	-2.4668	-2.5465	-2.6320	-2.6771	-2.7202	-2.7635	-2.8077	-2.8524	-2.8971	-2.9421
2660. U-U0	16363.	16366.	16746.	16747.	17127.	17292.	17457.	17622.	17713.	17713.
H-H0	35386.	35483.	31470.	31471.	38048.	40278.	41891.	43173.	44769.	46488.
(S-S0)/R	-2.4350	-2.5147	-2.6002	-2.6453	-2.6884	-2.7317	-2.7759	-2.8206	-2.8653	-2.9103
2680. U-U0	16512.	16515.	16895.	16896.	17275.	17440.	17605.	17770.	17861.	17861.
H-H0	35637.	35734.	31720.	31721.	38298.	40528.	42141.	43423.	45019.	46738.
(S-S0)/R	-2.4039	-2.4836	-2.5691	-2.6142	-2.6573	-2.7006	-2.7448	-2.7895	-2.8342	-2.8792
2700. U-U0	16662.	16665.	17045.	17046.	17425.	17590.	17755.	17920.	18011.	18011.
H-H0	35892.	35989.	31974.	31975.	38552.	40782.	42395.	43677.	45273.	47092.
(S-S0)/R	-2.3729	-2.4526	-2.5381	-2.5832	-2.6263	-2.6696	-2.7138	-2.7585	-2.8032	-2.8482
2720. U-U0	16812.	16815.	17195.	17196.	17575.	17740.	17905.	18070.	18161.	18161.
H-H0	36146.	36243.	32222.	32223.	38800.	41030.	42643.	43925.	45521.	47340.
(S-S0)/R	-2.3417	-2.4214	-2.5069	-2.5520	-2.5951	-2.6384	-2.6826	-2.7273	-2.7720	-2.8170
2740. U-U0	16962.	16965.	17345.	17346.	17725.	17890.	18055.	18220.	18311.	18311.
H-H0	36400.	36497.	32478.	32479.	39056.	41286.	42899.	44181.	45777.	47596.
(S-S0)/R	-2.3106	-2.3903	-2.4758	-2.5209	-2.5640	-2.6073	-2.6515	-2.6962	-2.7409	-2.7859
2760. U-U0	17112.	17115.	17495.	17496.	17875.	18040.	18205.	18370.	18461.	18461.
H-H0	36656.	36753.	32632.	32633.	39210.	41440.	43053.	44335.	45931.	47750.
(S-S0)/R	-2.2794	-2.3591	-2.4446	-2.4897	-2.5328	-2.5761	-2.6203	-2.6650	-2.7100	-2.7550
2780. U-U0	17262.	17265.	17645.	17646.	18025.	18190.	18355.	18520.	18611.	18611.
H-H0	36907.	37004.	32786.	32787.	39354.	41584.	43197.	44479.	46075.	47894.
(S-S0)/R	-2.2482	-2.3279	-2.4134	-2.4585	-2.5016	-2.5449	-2.5891	-2.6338	-2.6785	-2.7235
2800. U-U0	17412.	17415.	17795.	17796.	18175.	18340.	18505.	18670.	18761.	18761.
H-H0	37161.	37258.	32940.	32941.	39518.	41748.	43361.	44643.	46239.	48058.
(S-S0)/R	-2.2171	-2.2968	-2.3823	-2.4274	-2.4705	-2.5138	-2.5580	-2.6027	-2.6474	-2.6924
2820. U-U0	17562.	17565.	17945.	17946.	18325.	18490.	18655.	18820.	18911.	18911.
H-H0	37415.	37512.	33102.	33103.	39700.	41930.	43543.	44825.	46421.	48240.
(S-S0)/R	-2.1860	-2.2657	-2.3512	-2.3963	-2.4394	-2.4827	-2.5269	-2.5716	-2.6163	-2.6613
2840. U-U0	17712.	17715.	18095.	18096.	18475.	18640.	18805.	18970.	19061.	19061.
H-H0	37669.	37766.	33294.	33295.	39898.	42128.	43741.	45023.	46619.	48438.
(S-S0)/R	-2.1549	-2.2346	-2.3201	-2.3652	-2.4083	-2.4516	-2.4958	-2.5405	-2.5852	-2.6302
2860. U-U0	17862.	17865.	18245.	18246.	18625.	18790.	18955.	19120.	19211.	19211.
H-H0	37923.	38020.	33486.	33487.	40096.	42326.	43939.	45221.	46817.	48636.
(S-S0)/R	-2.1237	-2.2034	-2.2889	-2.3340	-2.3771	-2.4204	-2.4646	-2.5093	-2.5540	-2.5990
2880. U-U0	18012.	18015.	18395.	18396.	18775.	18940.	19105.	19270.	19361.	19361.
H-H0	38177.	38274.	33678.	33679.	40294.	42524.	44137.	45419.	47015.	48834.
(S-S0)/R	-2.0926	-2.1723	-2.2578	-2.3029	-2.3460	-2.3893	-2.4335	-2.4782	-2.5229	-2.5679
2900. U-U0	18162.	18165.	18545.	18546.	18925.	19090.	19255.	19420.	19511.	19511.
H-H0	38431.	38528.	33870.	33871.	40492.	42722.	44335.	45617.	47213.	49032.
(S-S0)/R	-2.0615	-2.1412	-2.2267	-2.2718	-2.3149	-2.3582	-2.4024	-2.4471	-2.4918	-2.5368
2920. U-U0	18312.	18315.	18695.	18696.	19075.	19240.	19405.	19570.	19661.	19661.
H-H0	38685.	38782.	34062.	34063.	40690.	42920.	44533.	45815.	47411.	49230.
(S-S0)/R	-2.0304	-2.1101	-2.1956	-2.2407	-2.2838	-2.3271	-2.3713	-2.4160	-2.4607	-2.5057
2940. U-U0	18462.	18465.	18845.	18846.	19225.	19390.	19555.	19720.	19811.	19811.
H-H0	38939.	39036.	34254.	34255.	40888.	43118.	44731.	46013.	47609.	49428.
(S-S0)/R	-2.0000	-2.0797	-2.1652	-2.2103	-2.2534	-2.2967	-2.3409	-2.3856	-2.4303	-2.4753
2960. U-U0	18612.	18615.	19000.	19001.	19380.	19545.	19710.	19875.	19966.	19966.
H-H0	39193.	39290.	34446.	34447.	41086.	43316.	44929.	46211.	47807.	49626.
(S-S0)/R	-1.9700	-2.0497	-2.1352	-2.1803	-2.2234	-2.2667	-2.3109	-2.3556	-2.4003	-2.4453
2980. U-U0	18762.	18765.	19145.	19146.	19525.	19690.	19855.	20020.	20111.	20111.
H-H0	39447.	39544.	34638.	34639.	41284.	43514.	45127.	46409.	48005.	49824.
(S-S0)/R	-1.9400	-2.0197	-2.1052	-2.1503	-2.1934	-2.2367	-2.2809	-2.3256	-2.3703	-2.4153
3000. U-U0	18912.	18915.	19295.	19296.	19675.	19840.	20005.	20170.	20261.	20261.
H-H0	39701.	39798.	34830.	34831.	41482.	43712.	45325.	46607.	48203.	49922.
(S-S0)/R	-1.9100	-1.9897	-2.0752	-2.1203	-2.1634	-2.2067	-2.2509	-2.2956	-2.3403	-2.3853

Table 4
Selected Hydrogen Properties and the Portions Thereof
Contributed by Each Energy Factor

DENSITY = 1.00 (AMAGAT)		VOLUME = 27428.00 (CC/MOLE)					
T (K)	P (ATM)	U/RT	H/RT	(S-S0)/R	CV/R	CP/R	
500.	1.83	2.452	3.453	1.589	2.520	3.519	TOTAL
		1.500	2.500	0.907	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	0.000	POTENTIAL
		0.952	0.952	0.602	1.019	1.019	VIBR/RBT
600.	2.20	2.464	3.465	1.969	2.528	3.528	TOTAL
		1.500	2.500	1.180	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	0.000	POTENTIAL
		0.964	0.964	0.789	1.028	1.028	VIBR/RBT
800.	2.93	2.484	3.484	2.700	2.563	3.563	TOTAL
		1.500	2.500	1.812	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	-0.000	POTENTIAL
		0.983	0.983	1.089	1.063	1.063	VIBR/RBT
1000.	3.65	2.506	3.507	3.279	2.633	3.633	TOTAL
		1.500	2.500	1.946	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	-0.000	POTENTIAL
		1.006	1.006	1.333	1.133	1.133	VIBR/RBT
1200.	4.39	2.535	3.536	3.767	2.728	3.727	TOTAL
		1.500	2.500	2.220	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	-0.000	POTENTIAL
		1.035	1.035	1.547	1.228	1.228	VIBR/RBT
1500.	5.49	2.589	3.590	4.393	2.884	3.884	TOTAL
		1.500	2.500	2.554	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	-0.000	POTENTIAL
		1.089	1.089	1.838	1.384	1.384	VIBR/RBT
2000.	7.32	2.693	3.694	5.256	3.120	4.120	TOTAL
		1.500	2.500	2.966	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	-0.000	POTENTIAL
		1.193	1.193	2.270	1.620	1.620	VIBR/RBT
2500.	9.15	2.794	3.798	5.973	3.302	4.302	TOTAL
		1.500	2.500	3.321	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	-0.000	POTENTIAL
		1.298	1.298	2.652	1.802	1.802	VIBR/RBT
3000.	10.98	2.894	3.895	6.588	3.441	4.441	TOTAL
		1.500	2.500	3.594	1.500	2.500	TRANSLATION
		0.000	0.001	0.000	0.000	-0.000	POTENTIAL
		1.394	1.394	2.993	1.941	1.941	VIBR/RBT

(Table continues)

Table 4 (Continued)

DENSITY = 10.00 (AMAGAT)
 VOLUME = 2242.80 (CC/MOLE)

T(K)	P(ATM)	U/RT	H/RT	(S-S0)/R	CV/M	CP/R	
500.	18.46	2.452	3.462	-0.801	2.521	3.520	TOTAL
		1.500	2.500	-1.396	1.500	2.500	TRANSLATION
		0.001	0.010	-0.007	0.002	0.001	POTENTIAL
		0.952	0.952	0.602	1.019	1.019	VIBR/ROT
600.	22.15	2.465	3.473	-0.341	2.529	3.520	TOTAL
		1.500	2.500	-1.123	1.500	2.500	TRANSLATION
		0.001	0.010	-0.007	0.002	0.000	POTENTIAL
		0.964	0.964	0.789	1.028	1.028	VIBR/ROT
800.	29.52	2.484	3.493	0.391	2.569	3.563	TOTAL
		1.500	2.500	-0.691	1.500	2.500	TRANSLATION
		0.001	0.010	-0.007	0.002	-0.000	POTENTIAL
		0.983	0.983	1.089	1.064	1.063	VIBR/ROT
1000.	36.89	2.507	3.515	0.970	2.639	3.632	TOTAL
		1.500	2.500	-0.386	1.500	2.500	TRANSLATION
		0.001	0.010	-0.006	0.002	-0.001	POTENTIAL
		1.006	1.006	1.333	1.133	1.133	VIBR/ROT
1200.	44.26	2.536	3.544	1.459	2.729	3.727	TOTAL
		1.500	2.500	-0.083	1.500	2.500	TRANSLATION
		0.001	0.009	-0.006	0.002	-0.001	POTENTIAL
		1.035	1.035	1.547	1.228	1.228	VIBR/ROT
1500.	55.31	2.590	3.598	2.084	2.806	3.803	TOTAL
		1.500	2.500	0.252	1.500	2.500	TRANSLATION
		0.001	0.009	-0.006	0.002	-0.001	POTENTIAL
		1.089	1.089	1.838	1.364	1.364	VIBR/ROT
2000.	73.77	2.695	3.702	2.948	3.121	4.119	TOTAL
		1.500	2.500	0.683	1.500	2.500	TRANSLATION
		0.001	0.009	-0.005	0.001	-0.001	POTENTIAL
		1.193	1.193	2.270	1.620	1.620	VIBR/ROT
2500.	92.13	2.799	3.806	3.665	3.303	4.300	TOTAL
		1.500	2.500	1.018	1.500	2.500	TRANSLATION
		0.001	0.009	-0.005	0.001	-0.001	POTENTIAL
		1.298	1.298	2.652	1.802	1.802	VIBR/ROT
3000.	110.52	2.895	3.902	4.280	3.442	4.439	TOTAL
		1.500	2.500	1.292	1.500	2.500	TRANSLATION
		0.001	0.008	-0.005	0.001	-0.001	POTENTIAL
		1.394	1.394	2.993	1.941	1.941	VIBR/ROT

(Table continues)

Table 4 (Continued)

DENSITY = 100.00 (AMAGAT)
 VOLUME = 224.28 (CC/MOLE)

T(K)	P(ATM)	U/RT	H/RT	(S-S0)/R	CV/H	CP/R	
500.	200.40	2.459	3.554	-3.181	2.538	3.528	TOTAL
		1.500	2.500	-3.699	1.500	2.500	TRANSLATION
		0.007	0.102	-0.085	0.019	0.009	POTENTIAL
		0.952	0.952	0.602	1.019	1.019	VIBR/ROT
600.	240.14	2.473	3.567	-2.718	2.546	3.532	TOTAL
		1.500	2.500	-3.425	1.500	2.500	TRANSLATION
		0.009	0.103	-0.081	0.018	0.004	POTENTIAL
		0.964	0.964	0.789	1.028	1.028	VIBR/ROT
800.	319.28	2.495	3.585	-1.981	2.581	3.562	TOTAL
		1.500	2.500	-2.994	1.500	2.500	TRANSLATION
		0.011	0.102	-0.076	0.018	-0.001	POTENTIAL
		0.983	0.983	1.089	1.063	1.063	VIBR/ROT
1000.	398.08	2.518	3.606	-1.399	2.650	3.629	TOTAL
		1.500	2.500	-2.659	1.500	2.500	TRANSLATION
		0.012	0.100	-0.072	0.017	-0.004	POTENTIAL
		1.006	1.006	1.333	1.133	1.133	VIBR/ROT
1200.	476.62	2.548	3.633	-0.907	2.744	3.721	TOTAL
		1.500	2.500	-2.385	1.500	2.500	TRANSLATION
		0.013	0.099	-0.069	0.016	-0.007	POTENTIAL
		1.035	1.035	1.547	1.228	1.228	VIBR/ROT
1500.	594.05	2.603	3.685	-0.279	2.900	3.876	TOTAL
		1.500	2.500	-2.051	1.500	2.500	TRANSLATION
		0.014	0.096	-0.066	0.016	-0.009	POTENTIAL
		1.089	1.089	1.838	1.384	1.384	VIBR/ROT
2000.	789.00	2.707	3.786	0.589	3.135	4.109	TOTAL
		1.500	2.500	-1.619	1.500	2.500	TRANSLATION
		0.014	0.092	-0.061	0.015	-0.010	POTENTIAL
		1.193	1.193	2.270	1.620	1.620	VIBR/ROT
2500.	983.24	2.812	3.887	1.300	3.316	4.290	TOTAL
		1.500	2.500	-1.285	1.500	2.500	TRANSLATION
		0.014	0.089	-0.058	0.014	-0.011	POTENTIAL
		1.298	1.298	2.652	1.802	1.802	VIBR/ROT
3000.	1176.93	2.908	3.980	1.926	3.454	4.429	TOTAL
		1.500	2.500	-1.011	1.500	2.500	TRANSLATION
		0.014	0.086	-0.056	0.014	-0.012	POTENTIAL
		1.394	1.394	2.993	1.941	1.941	VIBR/ROT

(Table continues)

Table 4 (Continued)

DENSITY = 500.00 (AMAGAT)							
VOLUME = 44.86 (CC/MOLE)							
T(K)	P(ATM)	U/R _T	H/R _T	(S-S ₀)/R	CV/R	CP/R	
500.	1473.47	2.496	4.107	-5.185	2.640	3.634	TOTAL
		1.500	2.500	-5.388	1.500	2.500	TRANSLATION
		0.045	0.654	-0.479	0.121	0.115	POTENTIAL
		0.952	0.952	0.602	1.019	1.019	VIBR/RBT
600.	1754.64	2.921	4.119	-4.703	2.644	3.615	TOTAL
		1.500	2.500	-5.035	1.500	2.500	TRANSLATION
		0.075	0.654	-0.458	0.116	0.087	POTENTIAL
		0.964	0.964	0.789	1.028	1.028	VIBR/RBT
800.	2303.84	2.954	4.128	-3.940	2.672	3.615	TOTAL
		1.500	2.500	-4.603	1.500	2.500	TRANSLATION
		0.071	0.645	-0.425	0.109	0.092	POTENTIAL
		0.983	0.983	1.089	1.063	1.063	VIBR/RBT
1000.	2840.07	2.984	4.136	-3.337	2.736	3.664	TOTAL
		1.500	2.500	-4.268	1.500	2.500	TRANSLATION
		0.078	0.630	-0.402	0.103	0.091	POTENTIAL
		1.006	1.006	1.333	1.133	1.133	VIBR/RBT
1200.	3366.65	2.616	4.150	-2.831	2.826	3.744	TOTAL
		1.500	2.500	-3.995	1.500	2.500	TRANSLATION
		0.082	0.615	-0.383	0.099	0.016	POTENTIAL
		1.035	1.035	1.947	1.228	1.228	VIBR/RBT
1500.	4142.75	2.673	4.183	-2.184	2.978	3.886	TOTAL
		1.500	2.500	-3.460	1.500	2.500	TRANSLATION
		0.085	0.594	-0.362	0.093	0.002	POTENTIAL
		1.089	1.089	1.838	1.384	1.384	VIBR/RBT
2000.	5489.27	2.779	4.258	-1.295	3.287	4.107	TOTAL
		1.500	2.500	-3.229	1.500	2.500	TRANSLATION
		0.086	0.564	-0.336	0.087	-0.012	POTENTIAL
		1.193	1.193	2.270	1.620	1.620	VIBR/RBT
2500.	6651.34	2.883	4.338	-0.559	3.384	4.281	TOTAL
		1.500	2.500	-2.894	1.500	2.500	TRANSLATION
		0.086	0.548	-0.317	0.082	-0.021	POTENTIAL
		1.298	1.298	2.652	1.802	1.802	VIBR/RBT
3000.	7875.26	2.978	4.413	0.070	3.519	4.414	TOTAL
		1.500	2.500	-2.620	1.500	2.500	TRANSLATION
		0.085	0.520	-0.302	0.078	-0.027	POTENTIAL
		1.394	1.394	2.993	1.941	1.941	VIBR/RBT

(Table continues)

Table 4 (Continued)

DENSITY = 1000.00 (AMAGAT)
 VOLUME = 22.43 (CC/MOLE)

T(K)	P(ATM)	U/R	W/R	(S-S ₀)/R	CV/R	CP/R	
500.	5022.73	2.570	5.325	-6.526	2.860	3.946	TOTAL
		1.500	2.500	-6.001	1.500	2.500	TRANSLATION
		0.127	1.873	-1.177	0.340	0.426	POTENTIAL
		0.952	0.952	0.662	1.019	1.019	VIBR/RBT
600.	5924.50	2.625	5.324	-6.005	2.851	3.876	TOTAL
		1.500	2.500	-5.728	1.500	2.500	TRANSLATION
		0.161	1.860	-1.066	0.323	0.348	POTENTIAL
		0.964	0.964	0.789	1.028	1.028	VIBR/RBT
800.	7632.92	2.682	5.289	-5.185	2.858	3.811	TOTAL
		1.500	2.500	-5.296	1.500	2.500	TRANSLATION
		0.198	1.866	-0.977	0.295	0.247	POTENTIAL
		0.983	0.983	1.069	1.063	1.063	VIBR/RBT
1000.	9250.74	2.721	5.250	-4.543	2.987	3.819	TOTAL
		1.500	2.500	-4.962	1.500	2.500	TRANSLATION
		0.215	1.744	-0.914	0.274	0.186	POTENTIAL
		1.006	1.006	1.333	1.133	1.133	VIBR/RBT
1200.	10803.76	2.758	5.219	-4.006	2.985	3.871	TOTAL
		1.500	2.500	-4.688	1.500	2.500	TRANSLATION
		0.224	1.684	-0.866	0.257	0.144	POTENTIAL
		1.035	1.035	1.547	1.228	1.228	VIBR/RBT
1500.	13044.09	2.817	5.194	-3.326	3.126	3.985	TOTAL
		1.500	2.500	-4.353	1.500	2.500	TRANSLATION
		0.228	1.605	-0.810	0.239	0.101	POTENTIAL
		1.089	1.089	1.838	1.384	1.384	VIBR/RBT
2000.	16609.46	2.921	5.191	-2.397	3.336	4.178	TOTAL
		1.500	2.500	-3.922	1.500	2.500	TRANSLATION
		0.228	1.498	-0.745	0.217	0.058	POTENTIAL
		1.193	1.193	2.270	1.620	1.620	VIBR/RBT
2500.	20027.49	3.022	5.211	-1.634	3.503	4.333	TOTAL
		1.500	2.500	-3.587	1.500	2.500	TRANSLATION
		0.224	1.414	-0.698	0.201	0.032	POTENTIAL
		1.298	1.298	2.652	1.802	1.802	VIBR/RBT
3000.	23339.58	3.113	5.239	-0.983	3.630	4.455	TOTAL
		1.500	2.500	-3.314	1.500	2.500	TRANSLATION
		0.219	1.386	-0.663	0.190	0.014	POTENTIAL
		1.394	1.394	2.993	1.941	1.941	VIBR/RBT

(Table continues)

Table 4 (Continued)

DENSITY = 1500.00 (AMAGAT)
VOLUME = 14.95 (CC/MOLE)

T(K)	P(ATM)	U/RT	H/RT	(S-S ₀)/R	CV/R	CP/R	
500.	13741.25	2.744	7.752	-7.647	3.288	4.554	TOTAL
		1.500	2.500	-6.467	1.500	2.500	TRANSLATION
		0.293	4.300	-2.043	0.768	1.034	POTENTIAL
		0.952	0.952	0.602	1.019	1.019	VIBR/ROT
600.	16014.26	2.831	7.694	-7.252	3.241	4.379	TOTAL
		1.500	2.500	-6.133	1.500	2.500	TRANSLATION
		0.367	4.231	-1.907	0.714	0.852	POTENTIAL
		0.954	0.954	0.729	1.028	1.028	VIBR/ROT
800.	20146.93	2.926	7.515	-6.328	3.190	4.182	TOTAL
		1.500	2.500	-5.782	1.500	2.500	TRANSLATION
		0.442	4.031	-1.715	0.627	0.619	POTENTIAL
		0.983	0.983	1.089	1.063	1.063	VIBR/ROT
1000.	23905.11	2.979	7.334	-5.616	3.198	4.111	TOTAL
		1.500	2.500	-5.367	1.500	2.500	TRANSLATION
		0.473	3.829	-1.582	0.565	0.478	POTENTIAL
		1.006	1.006	1.333	1.133	1.133	VIBR/ROT
1200.	27489.02	3.019	7.181	-5.029	3.246	4.112	TOTAL
		1.500	2.500	-5.094	1.500	2.500	TRANSLATION
		0.484	3.646	-1.483	0.519	0.384	POTENTIAL
		1.035	1.035	1.547	1.228	1.228	VIBR/ROT
1500.	32330.88	3.074	7.002	-4.294	3.392	4.175	TOTAL
		1.500	2.500	-4.759	1.500	2.500	TRANSLATION
		0.486	3.413	-1.373	0.468	0.291	POTENTIAL
		1.089	1.089	1.838	1.384	1.384	VIBR/ROT
2000.	39932.48	3.167	6.805	-3.384	3.532	4.317	TOTAL
		1.500	2.500	-4.327	1.500	2.500	TRANSLATION
		0.474	3.112	-1.247	0.412	0.197	POTENTIAL
		1.193	1.193	2.270	1.620	1.620	VIBR/ROT
2500.	47032.01	3.255	6.683	-2.500	3.677	4.444	TOTAL
		1.500	2.500	-3.993	1.500	2.500	TRANSLATION
		0.457	2.885	-1.159	0.379	0.142	POTENTIAL
		1.298	1.298	2.652	1.802	1.802	VIBR/ROT
3000.	53784.35	3.335	6.602	-1.819	3.789	4.546	TOTAL
		1.500	2.500	-3.719	1.500	2.500	TRANSLATION
		0.441	2.708	-1.093	0.348	0.105	POTENTIAL
		1.394	1.394	2.993	1.941	1.941	VIBR/ROT

(Table continues)

Table 4 (Continued)

DENSITY = 2000.00 (AMAG/T)
 VOLUME = 11.21 (CC/MOLE)

T(K)	P(ATM)	U/RT	W/RT	(S-SQ)/R	CV/R	CP/R	
500.	36522.68	3.108	13.096	-9.507	4.197	5.733	TOTAL
		1.500	2.500	-6.694	1.500	2.500	TRANSLATION
		0.656	9.638	-3.415	1.678	2.213	POTENTIAL
		0.957	0.952	0.602	1.019	1.019	VIBR/ROT
600.	41888.25	3.276	12.816	-8.756	4.037	5.317	TOTAL
		1.500	2.500	-6.421	1.500	2.500	TRANSLATION
		0.812	9.353	-3.124	1.510	1.790	POTENTIAL
		0.964	0.964	0.789	1.028	1.028	VIBR/ROT
800.	51074.86	3.436	12.161	-7.628	3.817	4.828	TOTAL
		1.500	2.500	-5.989	1.500	2.500	TRANSLATION
		0.952	8.877	-2.727	1.254	1.265	POTENTIAL
		0.983	0.983	1.089	1.063	1.063	VIBR/ROT
1000.	58959.29	3.500	11.558	-6.789	3.714	4.592	TOTAL
		1.500	2.500	-5.655	1.500	2.500	TRANSLATION
		0.994	8.052	-2.467	1.081	0.959	POTENTIAL
		1.006	1.006	1.333	1.133	1.133	VIBR/ROT
1200.	66024.48	3.533	11.052	-6.115	3.687	4.491	TOTAL
		1.500	2.500	-5.381	1.500	2.500	TRANSLATION
		0.998	7.517	-2.281	0.940	0.763	POTENTIAL
		1.035	1.035	1.547	1.228	1.228	VIBR/ROT
1500.	75616.20	3.566	10.455	-5.290	3.718	4.459	TOTAL
		1.500	2.500	-5.046	1.500	2.500	TRANSLATION
		0.977	6.866	-2.082	0.834	0.575	POTENTIAL
		1.089	1.089	1.838	1.384	1.384	VIBR/ROT
2000.	89910.02	3.617	9.760	-4.286	3.824	4.516	TOTAL
		1.500	2.500	-4.615	1.500	2.500	TRANSLATION
		0.924	6.067	-1.861	0.704	0.396	POTENTIAL
		1.193	1.193	2.270	1.620	1.620	VIBR/ROT
2500.	102878.64	3.669	9.293	-3.342	3.926	4.596	TOTAL
		1.500	2.500	-4.280	1.500	2.500	TRANSLATION
		0.871	5.495	-1.713	0.624	0.294	POTENTIAL
		1.298	1.298	2.652	1.882	1.882	VIBR/ROT
3000.	114976.53	3.719	8.956	-2.619	4.009	4.689	TOTAL
		1.500	2.500	-4.007	1.500	2.500	TRANSLATION
		0.825	5.063	-1.605	0.568	0.228	POTENTIAL
		1.394	1.394	2.993	1.941	1.941	VIBR/ROT

Appendix A

MOLECULAR POTENTIAL CORRECTION TO THERMODYNAMIC PROPERTIES

The purpose of this appendix is to develop the contributions of a dense gas to the thermodynamic properties that are due to the potential energy between the molecules. The starting point is the following equation which links classical and statistical thermodynamics:

$$P = RT \left(\frac{\partial}{\partial v} \ln Q \right)_T \quad (\text{A1})$$

or

$$\frac{Pv}{RT} = v \left(\frac{\partial}{\partial v} \ln Q \right)_T \quad (\text{A2})$$

where Q is the total partition function.

Rowlinson* has suggested the following equation of state for dense gases:

$$\frac{Pv}{RT} = Z = \frac{1 + \xi + \xi^2}{(1 - \xi)^3} \quad (\text{A3})$$

where

$$\xi = \frac{b_m}{4v} z^{1/4} \left[1 + \frac{1}{12} F(z) \right]^3$$

in which

$$z = \frac{\epsilon}{kT}$$

and

$$F(z) = \gamma - \sum_{l=1}^{\infty} \frac{\left(\frac{l}{2} - 1\right)! (2\sqrt{z})^l}{l!}$$

with γ , being Euler's constant.

The volume dependent terms in the partition function are due to the translational and potential energy of the molecule. The contribution of the potential energy alone can be found by subtracting from the compressibility the contribution of the translational energy, which is a constant and equal to one. Then, by substituting Eq. (A3) into Eq. (A2) and integrating, the partition function associated with the potential energy (denoted by the subscript p) may be obtained as follows:

*J. S. Rowlinson, "An Equation of State of Gases at High Temperatures and Densities," Mol. Phys. 7(No. 14):349-361 (1963-1964).

$$Z-1 = \frac{(4-2\xi+\xi^2)\xi}{(1-\xi)^3} = v \left(\frac{\partial}{\partial v} \ln Q_p \right)_T = -\xi \left(\frac{d}{d\xi} \ln Q_p \right)_T \quad (\text{A4})$$

since

$$\frac{d\xi}{\xi} = -v \frac{dv}{v} - \frac{dv}{v}$$

thus,

$$\left(\frac{dv}{v} \right)_T = -\frac{d\xi}{\xi}$$

Then integrating Eq. (A4):

$$\int_1^{Q_p} \frac{1}{Q_p} \ln Q_p = - \int_0^\xi \frac{4-2\xi+\xi^2}{(1-\xi)^3} d\xi \quad (\text{A5})$$

the results are

$$\ln Q_p = \ln(1-\xi) - \frac{3}{2(1-\xi)^2} + \frac{3}{2} \quad (\text{A6})$$

or

$$Q_p = (1-\xi)e^{-3/2(1-\xi)^{-2} + 3/2} \quad (\text{A7})$$

The total partition function can now be obtained by multiplying Q_p by those factors associated with the other types of energy to be considered.

The contribution to the thermodynamic properties of a dense gas due to the potential energy between the molecules can now be obtained using the following statistical thermodynamic equations:

$$\frac{u_p}{RT} = \left(\frac{\partial \ln Q_p}{\partial \ln T} \right)_v = \alpha(Z-1) \quad (\text{A8})$$

where

$$\alpha = \frac{1}{4} \left[1 - \frac{G(x)}{\left(1 + \frac{F(x)}{12} \right)} \right]$$

and

$$G(x) = -x \frac{dF}{dx}$$

$$\frac{h_p}{RT} = \frac{u_p}{RT} + \left(\frac{P_p}{RT} - 1 \right) = (\alpha+1)(Z-1) \quad (\text{A9})$$

$$\frac{s_p}{RT} = \frac{u_p}{RT} + \ln Q_p = \alpha(Z-1) - \frac{3}{2(1-\xi)^2} + \frac{3}{2} + \ln(1-\xi) \quad (\text{A10})$$

$$\frac{c_{v,p}}{R} = \frac{1}{R} \left(\frac{\partial u_p}{\partial T} \right)_v = \phi(Z-1) \left(1 + D\phi - \frac{\phi Z Z'}{Z-1} \right), \quad (\text{A11})$$

where

$$D\phi = \frac{T}{\phi} \frac{d\phi}{dT}$$

and

$$Z' = \frac{\xi}{Z} \frac{dZ}{d\xi},$$

and

$$\frac{c_{p,p} - c_{v,p}}{R} = \frac{1}{R} \left[P + \left(\frac{\partial u}{\partial v} \right)_T \right] \left[\left(\frac{\partial v}{\partial T} \right)_p - \frac{R}{P} \right] = \frac{Z(1-\phi Z')^2}{1+Z'} - 1. \quad (\text{A12})$$

Appendix B

GRAPHS OF SELECTED THERMODYNAMIC PROPERTIES OF HYDROGEN

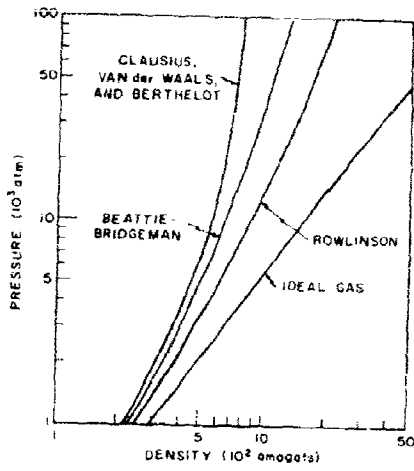


Fig. B1 - Comparison of Rowlinson equation of state with other well-known equations of state with initial gas state of 16 atm and 290°K

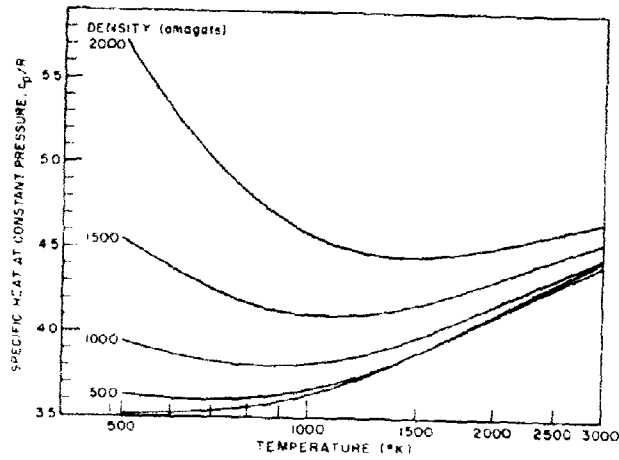


Fig. B2 - Specific heat at constant pressure vs temperature for constant density

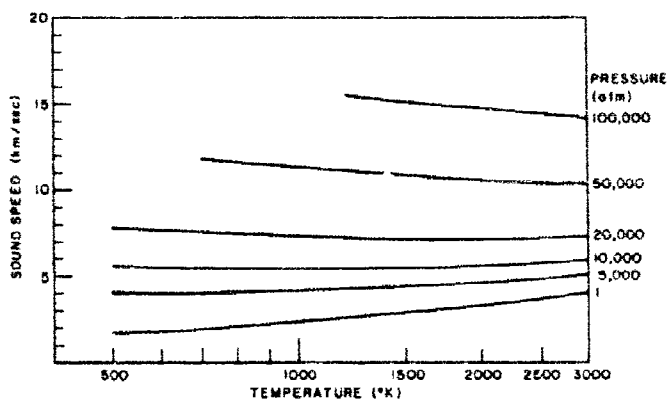


Fig. B3 - Sound speed vs temperature
for constant pressure

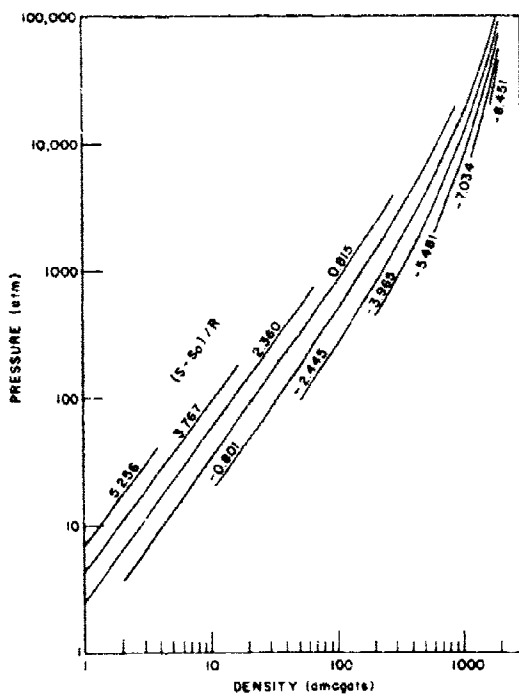


Fig. B4 - Pressure vs density
for constant entropy

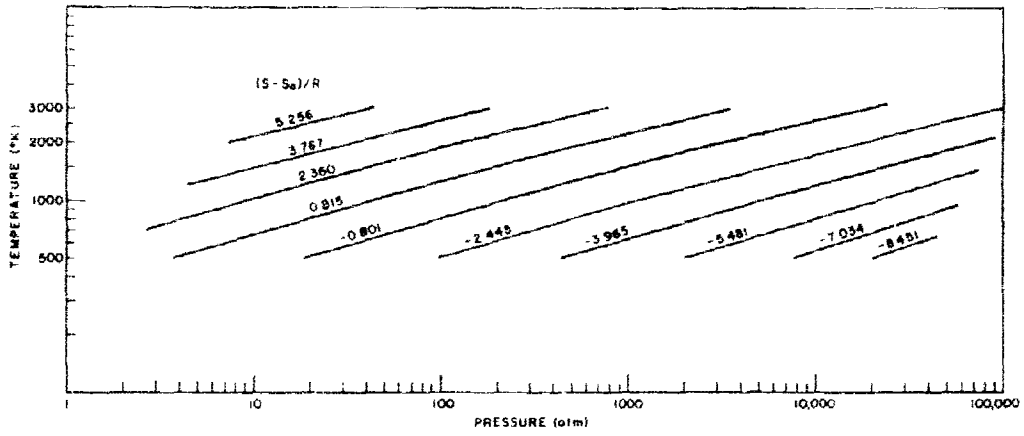


Fig. B5 - Temperature vs pressure for constant entropy

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The partition function corresponding to an equation of state for a high-temperature, high-density gas suggested by J. S. Rowlinson has been derived. The equations for selected thermodynamic properties of the gas are obtained from this partition function using statistical thermodynamics. These equations are used to calculate results for the case of hydrogen in the range of temperature between 500°K and 3000°K and in the range of density between 1 and 2000 amagats.			

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49

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