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COMPONENTS OF A HYDROGEN PLASMA INCLUDING MINOR SPECIES

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ABSTRACT

Tables and graphs of the number densities of hydrogen atoms (H), protons (H^+), free electrons (e^-), hydrogen molecules (H_2), negative hydrogen ions (H^-), hydrogen diatomic molecular ions (H_2^+), and hydrogen triatomic molecular ions (H_3^+) in a hydrogen gas or plasma in thermodynamic equilibrium were computed for temperatures from 300 to 40 000 K and pressures from 1.01325×10^5 to 1.01325×10^8 N/m^2 (1 to 1000 atm) except for a small, high-density region. For temperatures above 2000 K, the Debye-Hückel approximation was employed. Morse potentials are given for all singly excited attractive states of H_2 with principal quantum numbers to 17. A FORTRAN IV computer program for computing number densities and other properties of a hydrogen plasma is included.

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APPENDIXES

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SUMMARY

Tables and graphs of the number densities of hydrogen atoms (H), protons (H^+), free electrons (e^-), hydrogen molecules (H_2), negative hydrogen ions (H^-), hydrogen diatomic molecular ions (H_2^+), and hydrogen triatomic molecular ions (H_3^+) in a hydrogen gas or plasma in thermodynamic equilibrium were computed for temperatures from 300 to 40 000 K and pressures from 1.01325×10^5 to 1.01325×10^8 newtons per square meter (1 to 1000 atm) except for a small, high-density region. For temperatures above 2000 K, the Debye-Hückel approximation was employed. The ion H_3^+ had not been included in previous calculations and was found to cause large increases in e^- and H^- number densities at small degrees of ionization. The results presented in this report are believed to be the most accurate available. They are particularly applicable to calculating optical absorption coefficients. Also given are Morse potentials for all singly excited attractive states of H_2 with principal quantum numbers to 17.

A computer program in FORTRAN IV for computing number densities and other properties of a hydrogen plasma with or without coulomb interactions between free particles is presented. Sample problems and a flow diagram are also included.

INTRODUCTION

In high-temperature propulsion devices such as gaseous-core nuclear rockets, the dominant mechanism of heat transfer is radiant energy exchange between volumes of plasma and between the plasma and the wall. To calculate such heat transfer, it is necessary to know the opacity of the plasma. For a hydrogen plasma under many conditions, minor species make major contributions to the opacity, so their number densities must be known.

In past work (refs. 1 to 6) a wide variety of assumptions has been made, some of which were later shown to be invalid, and in no case were the hydrogen triatomic molecular ion (H_3^+) or excited electronic states of the hydrogen molecule (H_2) (designated H_2^* in this report) included. This investigation was conducted to provide more accurate estimates of number densities for hydrogen for temperatures between 300 and 40 000 K and pressures between 1.01325×10^5 and 1.01325×10^8 newtons per square meter (1 to 1000 atm). The species included above 2000 K were the hydrogen atom (H), the proton (H^+), the free electron (e^-), the negative hydrogen ion (H^-), the hydrogen diatomic molecular ion (H_2^+), H_2 (including H_2^*), and H_3^+. It was not feasible to estimate virial coefficients for all the species, so all intermolecular forces involving neutral species were neglected. This necessitated excluding a high-density region near 300 K and 10^8 newtons per square meter from the investigation.

One of the objects of the investigation was to find the effect of including H_3^+ on calculated number densities of e^- and H^-. Once this is known, the effect of H_3^+ on calculated electrical conductivity and opacity can be obtained.

ANALYSIS

The calculation of number densities over the wide range of 40 000 to 300 K necessitated three analyses to prevent major underflows in the digital computer program. The range from 40 000 to 2000 K was designated "high" temperature, 2000 to 1300 K was "medium" temperature, and 1300 to 300 K was "low" temperature. In all three analyses, values of the fundamental constants were obtained from reference 7.

High Temperature (2000 to 40 000 K)

The equilibrium components of the plasma were calculated in this range by minimizing the Gibbs free energy G of a closed, neutral system at constant temperature T and pressure p(ref. 8). (Symbols are given in appendix A.) Hence, equations for Gibbs free energy, pressure, charge conservation, and proton conservation were required and are given in this section. The partition functions needed to calculate the Gibbs free energy are also given.

Assumptions and restrictions. - The assumptions and restrictions utilized in the high-temperature analysis are as follows:

(1) The species $H(H^\ddagger$ and $H^*)$, H^+, e^-, $H_2(H_2^\ddagger$ and $H_2^*)$, H^-, H_2^+, and H_3^+ were included, where $H^\ddagger$ and $H_2^\ddagger$ are the ground electronic states of H and H_2, respectively, and H^* is all excited electronic states of H collectively.

(2) The plasma was treated as an ideal gas except for coulomb interactions between free charged particles, which were treated by the Debye-Hückel approximation.

(3) No shifts of energy levels of excited electronic states relative to ground electronic states were considered. (These shifts are observed to be small (refs. 9 and 10), and no one has correlated the observed shifts for H^* (ref. 9) with a theory whose assumptions would be valid for the conditions of the experiment.)

(4) Only singly excited electronic states of H_2 were considered. (Most doubly excited electronic states of H_2 have negligible number densities.)

(5) The free electrons were nondegenerate (i.e., they had a Boltzmann distribution of velocities).

(6) The contribution of photons to the pressure was neglected.

(7) Nuclear spin was taken into account in a consistent manner (i.e., it was not included in calculating degeneracies of atoms and atomic ions and was accounted for in molecules and molecular ions by using a symmetry number (ref. 11)). An additional refinement consistent with this method was included for $H_2^{\ddagger}$ and H_2^+.

Gibbs free energy. - To obtain the Debye-Hückel approximation for the Gibbs free energy of a plasma, it is first necessary to know the reciprocal Debye length, the excess Helmholtz free energy, and the excess pressure. For a plasma the reciprocal Debye length is

$$\kappa = \left(\frac{e^2}{\epsilon_0 kTV} \sum z_i^2 N_i\right)^{1/2} \tag{1}$$

where z_i is the net number of elementary charges on the particle (1, 0, or -1) and the summation is over all free particles. The excess Helmholtz free energy A_{ex} is the addition to the ideal-gas Helmholtz free energy resulting from coulomb interactions and, according to the Debye-Hückel theory (refs. 11 and 12), is

$$A_{ex} = -\frac{kTV\kappa^3}{12\pi} \tag{2}$$

Consequently, the excess pressure p_{ex} is

$$p_{ex} = -\left(\frac{\partial A_{ex}}{\partial V}\right)_{T,N_i} = -\frac{kT\kappa^3}{24\pi} \tag{3}$$

The excess Gibbs free energy is then

$$G_{ex} = A_{ex} + p_{ex}V = - \frac{kTV\kappa^3}{8\pi} \tag{4}$$

From reference 11 and equation (4) the total Gibbs free energy of a hydrogen plasma is

$$G = \sum_{i=1}^{7} N_i \mu_{i, id} - \frac{kTV\kappa^3}{8\pi} \tag{5}$$

where $\mu_{i, id}$ is the chemical potential for species i in an ideal gas mixture. In such an ideal mixture, the $\mu_{i, id}$ of one species is independent of the presence of all other species (ref. 11); thus, equation (5) becomes

$$G = -kT \sum_{i=1}^{7} N_i \ln \frac{Vq_i}{\Lambda_i N_i} - \frac{kTV\kappa^3}{8\pi} \tag{6}$$

where

$$\Lambda_i \equiv \left(\frac{h^2}{2\pi m_i kT}\right)^{3/2} \qquad i = 1, 2, \ldots, 7 \tag{7}$$

Equation (6) is the desired expression for the Gibbs free energy of a plasma.

Pressure. - The pressure is found from the ideal-gas law and equation (3) and is

$$p = \frac{kT}{V} \sum_{i=1}^{7} N_i - \frac{kT\kappa^3}{24\pi} \tag{8}$$

Charge conservation. - For a neutral plasma

$$N_3 + N_5 = N_2 + N_6 + N_7 \tag{9}$$

Proton conservation. - In a closed system the number of protons η' must be conserved, where

$$\eta' = N_1 + N_2 + 2N_4 + N_5 + 2N_6 + 3N_7 \tag{10}$$

Equilibrium. - For thermodynamic equilibrium, the eight variables N_i and V were simultaneously varied to minimize G (eq. (6)) subject to the constraints given by equations (8) to (10). The method for this, given in appendix B, gives the same result as using equations (8) to (10) in conjunction with a dissociative equilibrium equation for each of the reactions

$$H_2 \rightarrow 2H$$

$$H_3^+ \rightarrow H_2^+ + H$$

$$H^- \rightarrow H + e^-$$

$$H_2^+ \rightarrow H + H^+$$

and a Saha equation with lowering of the ionization potential (ref. 12) for the reaction

$$H \rightarrow H^+ + e^-$$

Internal partition functions. - In carrying out the minimization of G, values for q_i are required in equation (6). These values must all be referred to the energies of two reference states. First, however, the partition functions q_i' were calculated using the ground-state energy of each species as the reference.

For H atoms

$$q_1' = 2 + \sum_{n=2}^{17} F_n \varphi_n \tag{11}$$

where

$$\varphi_n \equiv 2n^2 e^{-hcT_e/kT} \tag{12}$$

and F_n is a cutoff factor given in appendix C. The summation is carried out through a principal quantum number n of 17 because F_n is 0 for larger n for all conditions in this report. For H^+, q_2' is 1. For e^-, q_3' is 2. The q_i' for H_2, H^-, H_2^+, and H_3^+ are given in subsequent paragraphs.

For H_2 there are contributions made by $H_2^\ddagger$ and H_2^*. The contribution of $H_2^\ddagger$ to the partition function of H_2 neglecting nuclear spin is obtained from equation (6) of reference 13 by substituting J for K and is

$$q'_{H_2^\ddagger} = \frac{g_e}{\sigma} \sum_v \sum_J (2J + 1) e^{-hc\left[G_v + f(v, J)\right]/kT} \tag{13}$$

Here g_e is 1, σ is 2, and the J summation includes metastable levels. For $H_2^\ddagger$ the rotational levels are spaced widely enough so the differences in nuclear spin degeneracies should be taken into account, at least near 300 K. Equation (13) then obviously becomes

$$q'_{H_2^\ddagger} = \sum_v \zeta_v \tag{14}$$

where

$$\zeta_v = \frac{g_e}{\sigma} e^{-hcG_v/kT} \left[\frac{3}{2} \sum_{\text{odd}\,J} (2J + 1) e^{-hcf(v, J)/kT} + \frac{1}{2} \sum_{\text{even}\,J} (2J + 1) e^{-hcf(v, J)/kT}\right] \tag{15}$$

Values of G_v were obtained from reference 14. Values of $f(v, J)$ were calculated by the Wentzel-Kramers-Brillouin approximation using the computer program in reference 13. The most reliable potential energy was used at each internuclear distance, namely, (1) from 0.37×10^{-10} to 0.40×10^{-10} meter the Kolos and Wolniewicz potential (ref. 15) was used, (2) from 0.41×10^{-10} to 3.00×10^{-10} meter the Rydberg-Klein-Rees potential of Spindler (ref. 14) was used, (3) from 3.01×10^{-10} to 5.29×10^{-10} meter the Kolos and Wolniewicz potential was used, and (4) from 5.55×10^{-10} to 25×10^{-10} meter the Hirschfelder and Löwdin potential (ref. 16) was used. Potential energies at internuclear distances not included in (1) to (4) were obtained by interpolation.

The partition function q'_4 for H_2 was obtained by adding the contributions of H_2^* to $q'_{H_2^\ddagger}$.

$$q'_4 = q'_{H_2^\ddagger} + \sum F_n \gamma_h \tag{16}$$

where the summation is over all singly excited electronic states H_2^* with n of 17 or less, where n is the principal quantum number of the excited electron in the small-internuclear-distance designation (ref. 17) and where

$$\gamma_h = \frac{8\pi^{1/2} g_e}{\sigma} \left(\frac{2\pi\mu kT}{h^2}\right)^{3/2} e^{-hc\tilde{T}/kT} \left[\frac{r_e^2 W_o(\theta)}{\beta} + \frac{2r_e W_I(\theta)}{\beta^2} + \frac{W_{II}(\theta)}{\beta^3}\right] R_h \tag{17}$$

and

$$R_h = \frac{ue^{-u/2}}{1 - e^{-u}}, \qquad u = \frac{hc\omega'}{kT}, \qquad \theta = \frac{kT}{hcD} \tag{18}$$

Equation (17) is a classical partition function with a vibrational quantum correction for a Morse vibrating rotator. It was obtained from equation (5) in reference 18 by multiplying by g_e and shifting the reference energy to that of the rotationless ground vibrational state of $H_2^\ddagger$. The constants $\tilde{T}$, r_e, β, D, and ω' were obtained as discussed in appendix D. Where available, experimental energy levels for n of 2 to 4 in the small-internuclear-distance designation were used in obtaining these constants (see appendix E and table I). Values of g_e, $\tilde{T}$, r_e, β, and D are given in table II.

The ground state of H^- is a $^1S_0$ state (ref. 19). Electronically excited states were neglected, so q_5' had the value 1.

The ground state of H_2^+ is a $^2\Sigma_g^+$ state, whereas the ground state of H_2 is a $^1\Sigma_g^+$ state. Because they both have the same nuclear spin statistics, q_6' is obtainable (ref. 20) from equations (14) and (15) by substituting q_6' for $q'_{H_2^\ddagger}$ and K for J. To avoid confusion later, ζ_v is replaced by Ω_v, so equations (14) and (15) become

$$q_6' = \sum_v \Omega_v \tag{19}$$

where

$$\Omega_v = \frac{g_e}{\sigma} e^{-hcG_v/kT} \left[\frac{3}{2} \sum_{\text{odd K}} (2K+1) e^{-hcf(v,K)/kT} + \frac{1}{2} \sum_{\text{even K}} (2K+1) e^{-hcf(v,K)/kT} \right] \tag{20}$$

The summations include metastable rotational levels. Excited electronic states of H_2^+ were neglected. Values for G_v were obtained from reference 21, and values for f were obtained from reference 13.

The partition function q_7' for H_3^+ was obtained from reference 13, where electronically excited states were neglected.

The atom $H^\ddagger$ and the free electron e^- were selected as the two reference states for the q_i. The shifts in reference energies from the values used for the q_i' result in the following relations:

$$\left.\begin{aligned} &q_1 = q'_1, \qquad q_2 = q'_2 e^{-hcI_1^{\ddagger}/kT}, \qquad q_3 = q'_3, \qquad q_4 = q'_4 e^{hcW_4^{\ddagger}/kT} \\ &q_5 = q'_5 e^{hcI_5/kT}, \qquad q_6 = q'_6 e^{-hc(I_1^{\ddagger}-W_6)/kT}, \qquad q_7 = q'_7 e^{-hc(I_1^{\ddagger}-W_7)/kT} \end{aligned}\right\} \tag{21}$$

Note that the lowering of the ionization potential due to coulomb interactions was omitted from equation (21) as this effect is already included in the last term of equation (6). Values for $I_1^{\ddagger}$, I_5, $W_4^{\ddagger}$, W_6, and W_7 are given in table III.

Medium Temperature (1300 to 2000 K)

In this range the high-temperature analysis was inapplicable because of major underflows in the computer. The degree of ionization was so small that the coulomb interaction between free charged particles was negligible and consequently could be neglected. The number densities of H^+ and H_2^+ were each less than 2×10^{-5} times the number density of H_3^+, so the first two could be neglected. The equilibrium components of the plasma were calculated by means of equilibrium constants, using partition functions from the previous section.

Assumptions and restrictions. - The assumptions and restrictions utilized in the medium-temperature analysis are as follows:

(1) Only the species $H(H^{\ddagger}$ and $H^*)$, e^-, $H_2(H_2^{\ddagger}$ and $H_2^*)$, H^-, and H_3^+ were included.

(2) The plasma was treated as an ideal gas.

(3) No shifts of energy levels of excited electronic states relative to ground electronic states were considered.

(4) Only singly excited electronic states of H_2 were considered.

(5) Nuclear spin was taken into account in the same way as in the high-temperature analysis.

Solution. - Let p'_o be an arbitrary reference pressure and define

$$s' \equiv \frac{p}{p'_o}, \qquad s'_i \equiv \frac{p_i}{p'_o} \qquad i = 1, 2, \ldots, 7 \tag{22}$$

For the reaction $2H \rightarrow H_2$ the equilibrium constant K_{p1} is (ref. 11)

$$\frac{s_4'}{s_1'^2} \equiv K_{p1} = \frac{kTq_4'}{\Lambda_4 p_o'}\left(\frac{kTq_1}{\Lambda_1 p_o'}\right)^{-2} e^{hcW_4^{\ddagger}/kT} \tag{23}$$

Define

$$\alpha_i \equiv N_o \Lambda_i T^{3/2} = N_o \left(\frac{h^2}{2\pi m_i k}\right)^{3/2} \qquad i = 1, 2, \ldots, 7 \tag{24}$$

Combining equations (23) and (24) gives

$$K_{p1} = \frac{RT^{5/2}q_4'}{\alpha_4 p_o'}\left(\frac{RT^{5/2}q_1}{\alpha_1 p_o'}\right)^{-2} e^{hcW_4^{\ddagger}/kT} \tag{25}$$

For medium temperatures and pressures between 1.01325×10^5 and 1.01325×10^8 newtons per square meter (1 to 1000 atm), s_1' and s_4' are much larger than s_3', s_5', and s_7'. Hence, $H(H^{\ddagger}$ and $H^*)$ and $H_2(H_2^{\ddagger}$ and $H_2^*)$ are treated as major species and e^-, H^-, and H_3^+ as minor species. Thus, dropping the last term in equation (8) gives

$$s' \approx s_1' + s_4' \tag{26}$$

which is Dalton's law for ideal gases. Combining equations (23) and (26) gives

$$s_1' \approx \frac{\left(4s'K_{p1} + 1\right)^{1/2} - 1}{2K_{p1}} \tag{27}$$

The value of s_4' may then be calculated from equation (26).

To find s_3', s_5', and s_7', the values of s_1' and s_4' from equations (27) and (26) are used together with appropriate equilibrium constants and the condition for electrical neutrality. For the reaction $(3/2)H_2 \rightarrow H_3^+ + e^-$

$$\frac{s_7's_3'}{s_4'^{3/2}} \equiv K_{p7} = \left(\frac{RT^{5/2}q_7'}{\alpha_7 p_o'}\right)\left(\frac{RT^{5/2}q_3}{\alpha_3 p_o'}\right)\left(\frac{RT^{5/2}q_4'}{\alpha_4 p_o'}\right)^{-3/2} e^{-hc\left[(3W_4^{\ddagger}/2) + I_1^{\ddagger} - W_7\right]/kT} \tag{28}$$

The dissociation energy W_7 is defined in table III. For the reaction $H + e^- \rightarrow H^-$

$$\frac{s'_5}{s'_1 s'_3} \equiv K_{p5} = \left(\frac{RT^{5/2} q'_5}{\alpha_5 p'_o}\right)\left(\frac{RT^{5/2} q_1}{\alpha_1 p'_o}\right)^{-1}\left(\frac{RT^{5/2} q_3}{\alpha_3 p'_o}\right)^{-1} e^{hcI_5/kT} \tag{29}$$

For electrical neutrality

$$s'_7 = s'_5 + s'_3 \tag{30}$$

From equations (28), (29), and (30)

$$s'_3 = \left(\frac{s'^{3/2}_4 K_{p7}}{K_{p5} s'_1 + 1}\right)^{1/2} \tag{31}$$

and s'_7 and s'_5 are found from equations (28) and (30). The number density of species i is given by $s'_i p'_o/kT$.

Low Temperature (300 to 1300 K)

In this range the medium-temperature analysis was inapplicable because it caused major underflows on the computer. All ionization and electronic excitation were negligible, and the number density $\hat{N}_1^{\ddagger}$ was much less than $\hat{N}_4^{\ddagger}$ for pressures from 1.01325×10^5 to 1.01325×10^8 newtons per square meter (1 to 1000 atm). The equilibrium components of the gas were calculated from the equilibrium constant K_{p1} given by equation (25).

Assumptions and restrictions. - The assumptions and restrictions utilized in the low-temperature analysis are as follows:

(1) Only the species $H^{\ddagger}$ and $H_2^{\ddagger}$ were included.

(2) The gas was treated as an ideal gas.

(3) Nuclear spin was taken into account in the same way as in the high-temperature analysis.

Solution. - The molecule $H_2^{\ddagger}$ was treated as the only major species, and the atom $H^{\ddagger}$ was treated as the minor species. Hence, $\hat{N}_4^{\ddagger} \approx \hat{N}$, and from equation (23) and the perfect-gas law

$$\hat{N}_1^{\ddagger} \approx \frac{1}{kT}\left(\frac{p'_o p}{K_{p1}}\right)^{1/2} \tag{32}$$

Computer Program

The high-, medium-, and low-temperature analyses were programmed in FORTRAN IV in a single program given in appendix B.

RESULTS AND DISCUSSION

In this section the rotational term values for $H_2^{\ddagger}$ are given. Compositions obtained using these term values are then presented. The effects on the composition of including or omitting H_3^+ and coulomb interactions between free charged particles are given. The accuracy of the compositions is discussed, and the compositions are compared with those obtained by other investigators.

Rotational Term Values for $H_2^{\ddagger}$

The calculated rotational term values f for $H_2^{\ddagger}$ are given in table IV (missing values indicate nonexistent states). These values agree to within 700 meters^{-1} with rotational term values calculated from wavelengths of lines measured by Herzberg and Howe (ref. 22). The values of f in table IV predict wave numbers of lines within 170 meters^{-1} of the values measured by Stoicheff (ref. 23), Fink, Wiggins, and Rank (ref. 24), and Herzberg (ref. 25). Table IV is also in excellent agreement with the calculations from first principles of Waech and Bernstein (ref. 26).

Components of Hydrogen Plasma

The number densities of species in a hydrogen plasma are given in tables V(a) to (d). The range of temperatures and pressures included in these tables is indicated by the area without crosshatching in figure 1. Typical cases in table V were checked to make sure they satisfied four different dissociative equilibrium equations and a Saha equation with lowering of the ionization potential (ref. 12). Number densities from tables V(a) and (d) are plotted in figures 2(a) and (b), respectively. By comparing figures 2(a) and (b), it is evident that higher pressure tends to inhibit dissociation and ionization, as expected.

Effect of H_3^+ on Composition, Electrical Conductivity, and Opacity

Of the partition functions of the seven species considered at high temperatures, the partition function of H_3^+ is least accurately known (ref. 13). Consequently, the effect of including or neglecting H_3^+ on the number densities of e^- and H^- was investigated. For small degrees of ionization, including H_3^+ substantially increased the number densities of e^- and H^-, as shown in figure 3 for a pressure of 1.01325×10^8 newtons per square meter (1000 atm). However, number densities of e^- and H^- are less dependent on the inclusion or neglect of H_3^+ at lower pressures. Including H_3^+ will thus increase the calculated electrical conductivity (through e^-) and opacity (through bremsstrahlung and H^- adsorption).

Effect of Coulomb Interactions Between Free Particles

Coulomb interactions between free particles reduce the pressure as shown by equation (8). The effect can be evaluated by calculating the coulomb compressibility

$$Z_c \equiv \frac{p}{kT \sum_{i=1}^{7} \hat{N}_i} \tag{33}$$

which is 1 for an ideal gas and less than 1 if coulomb interactions between free particles are considered. For the conditions in this report Z_c was never less than 0.92.

A much larger effect of coulomb interactions occurs with the number densities of certain species. The ratio of calculated number densities of H, e^-, and H^- with and without coulomb interactions between free particles is shown in figure 4 for a pressure of 1.01325×10^8 newtons per square meter (1000 atm). It is apparent that at this pressure coulomb interactions between free charged particles must be included in composition calculation if acceptable accuracy is to be achieved. However, at lower pressure the effect is smaller.

Accuracy of Composition

Based on the assumptions made and the constants used in the three analyses, the nonzero number densities in tables V(a) to (d) are accurate to four significant figures with two possible exceptions. At temperatures below about 2500 K the number densities of H_2^* and H^* may be too small because of a feature in the computer program designed to prevent major underflows. However, at these low temperatures these excited species are negligible anyhow. In any case, this possible discrepancy is less important than possible inaccuracies in the assumptions made and the constants used, which are discussed in the following paragraphs.

For consistency it was necessary to neglect all intermolecular forces involving neutral species. This caused serious inaccuracies in number densities at the highest densities, which occurred at low temperatures where only H and H_2 were significant. To evaluate these inaccuracies, number densities of H and H_2 were calculated from the relations and second and third virial coefficients of Fisher (ref. 27). In all cases the relative effect of the virial coefficients was larger on $\hat{N}_1$ than on $\hat{N}_4$. The inaccuracy in $\hat{N}_1$ when virial coefficients were neglected is shown in figure 1. As a result, temperatures and pressures where the inaccuracy in $\hat{N}_1$ exceeded 20 percent were excluded from this report (see fig. 1).

The only assumptions made that would be likely to cause inaccuracies exceeding 20 percent in the unshaded area in figure 1 pertained to electronically excited states of H_2, H, H_3^+, H_2^+, and H^-. The number density of H_2^* is possibly only accurate to within 50 percent because (1) metastable rotational states were neglected, (2) shifts in energy levels were neglected, (3) doubly excited states were neglected, and (4) the Bethe cutoff is somewhat arbitrary. However, it is doubtful if H_2^* contributes appreciably to the absorption coefficient of a hydrogen plasma, and H_2^* is certainly unimportant thermodynamically. The number density of H^* is possibly only accurate to within 50 percent at 40 000 K because (1) shifts in energy levels were neglected and (2) the Bethe cutoff is somewhat arbitrary. The number density of H^* should be much more accurate at appreciably lower temperatures. At 40 000 K there are probably appreciable inaccuracies in H_3^+, H_2^+, and H^- number densities because of the neglect of electronically excited states. The number densities of these species are negligible at this temperature, so the inaccuracies are academic. At appreciably lower temperatures the excited electronic states are unimportant.

There is a limit to the charged-particle density at which the Debye-Hückel theory is accurate. For a hydrogen plasma, the theory is believed valid provided (refs. 28 and 12)

$$r_c \equiv \frac{\kappa^2}{4\left[\pi\left(\hat{N}_2 + \hat{N}_3 + \hat{N}_5 + \hat{N}_6 + \hat{N}_7\right)\right]^{2/3}} < 1 \tag{34}$$

However, as r_c approaches 1, the accuracy can be expected to decrease (ref. 29). For the conditions in this report, r_c never exceeded 0.6.

The largest possible sources of error in this report were the constants and potential for H_3^+, which were used to calculate the partition function (ref. 13). These quantities were based on Conroy's calculations from first principles (ref. 30), which are believed to be reliable. However, there are no experimental vibrational frequencies or dissociation energy for H_3^+.

Comparison of Composition with Other Investigators

Calculated number densities for H_2 and e^- obtained in this report and by two other investigators are shown in figure 5. The number density of H_2 obtained from Krascella and Patch's results (ref. 1) was low at high temperatures because K_{p1} was extrapolated from lower temperatures. The number density of H_2 obtained from Rosenbaum and Levitt's results (ref. 2) was low at high temperature because metastable rotational states were neglected. The number density of e^- obtained from Krascella and Patch's results (ref. 1) was high because the lowering of the ionization potential was calculated from Ecker and Weizel's analysis (ref. 31), which was incorrect (ref. 32). The number density $\hat{N}_3$ of e^- obtained from Rosenbaum and Levitt's results was low because coulomb interactions between free charged particles were neglected. At the pressure for figure 5, H_3^+ does not affect $\hat{N}_3$ appreciably for the range of $\hat{N}_3$ shown therein.

CONCLUDING REMARKS

The number densities of the components of a hydrogen plasma including minor species were calculated. Coulomb interactions between free charged particles were considered for temperatures above 2000 K. Below this temperature they are insignificant. The hydrogen triatomic molecular ion (H_3^+), which had been neglected in previous calculations, was included and was found to increase the number densities of e^- and H^- substantially for small degrees of ionization. The largest possible source of error in this report was the constants for H_3^+, which have not been experimentally verified.[1] Because of the inclusion of minor species, the results of this report will be particularly useful for calculating optical absorption coefficients.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, July 9, 1968,
122-28-02-17-22.

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[1] Since this report was written, Leventhal and Friedman (J. Chem. Phys., vol. 49, no. 4, Aug. 15, 1968, pp. 1974-1975) have experimentally determined the dissociation energy of D_3^+. Allowing for differences in vibrational zero point energies of H_3^+ and D_3^+ and also H_2 and D_2, their results agree within the experimental error with the dissociation energy of H_3^+ used in reference 13 and in this report.

APPENDIX A

SYMBOLS

A	Helmholtz free energy, J
a_n, a_{n-1}, a_{n+1}	radius of electron orbit, m
a_o	first Bohr radius, m
C	excess of negative charges over positive charges, moles
c	speed of light, m/sec
D	Morse well depth, m^{-1} (see fig. 8)
$\underline{\mathscr{D}}$	correction column vector
$\mathscr{D}_i$ (i=01, 02, . . . , 05)	elements of $\underline{\mathscr{D}}$
d	correction to Dieke's (ref. 33) term values for triplet H_2^*, m^{-1}
e	charge of electron, C
F_n	cutoff factor
f, f(v, J), f(v, K)	rotational term values, m^{-1} (see fig. 8)
G	Gibbs free energy, J
G_v	vibrational term value, m^{-1} (see fig. 8)
g	reduced Gibbs free energy, moles
g_e	electronic degeneracy
H	hump height, m^{-1} (see figs. 8 and 9)
h	Planckś constant, J sec
I_e	clamped-nuclei ideal-gas ionization potential, m^{-1} (see fig. 8)
I, I_n, I_{n-1}, I_{n+1}	ideal-gas ionization potential (for rotationless ground vibrational states in the case of molecules), m^{-1} (see fig. 8)
ΔI	absolute value of change in ionization potential, m^{-1}
J	total angular momentum quantum number
K	quantum number for total angular momentum apart from electron spin
K_{p1}, K_{p5}, K_{p7}	equilibrium constants
k	Boltzmann constant, J/K

m_i $(i=1,2,\ldots,7)$	mass of species i, kg
$\hat{N}$	total number density, $1/m^3$
$\hat{N}_i$ $(i=1,2,\ldots,7)$	number density of species i, $1/m^3$
$\hat{N}_{1n}$	number density of H with principal quantum number n, $1/m^3$
N_i $(i=1,2,\ldots,7)$	number of particles of species i
N_o	Avogadro's number, 1/mole
n	principal quantum number
n^+	effective quantum number
n_i $(i=1,2,\ldots,7)$	moles of species i, moles
Δn_i $(i=1,2,\ldots,7)$	change in n_i, moles
$\Delta \ln n_i$ $(i=1,2,\ldots,7)$	change in natural logarithm of n_i
p	pressure, N/m^2
p_o', p_o	reference pressures, N/m^2
p_i $(i=1,2,\ldots,7)$	partial pressure of species i, N/m^2
q_i' $(i=1,2,\ldots,7)$	internal partition function of species i relative to ground electronic state (rotationless ground vibrational state in case of molecules and molecular ions)
$q'_{H_2^\ddagger}$	contribution of ground electronic state to q_4'
q_i $(i=1,2,\ldots,7)$	ideal-gas internal partition functions of species i relative to internal energy of e^- and $H^\ddagger$
R	universal gas constant, J/(mole)(K)
R_h	vibrational quantum correction
R_y	Rydberg constant, m^{-1}
r	internuclear distance, m
r_c	ratio of equivalent concentration to critical equivalent concentration
r_e	equilibrium internuclear distance, m
r_o	half the average distance between neighboring molecules, m
s'	nondimensionalized pressure, p/p_o'
s_i' $(i=1,2,\ldots,7)$	nondimensionalized partial pressure, p_i/p_o'

s	nondimensionalized pressure, p/p_o
T	temperature, K
$\tilde{T}$	energy difference between bottom of potential well of state of H_2^* and rotationless ground vibrational state of $H_2^\ddagger$, m^{-1} (see fig. 8)
T^+	energy difference between rotationless ground vibrational states of H_2^* and $H_2^\ddagger$, m^{-1} (see fig. 8)
T_e	electronic term value for H^* relative to $H^\ddagger$, m^{-1}
U(r)	potential energy measured from rotationless ground vibrational state of $H_2^\ddagger$, m^{-1}
u	dimensionless fundamental vibration frequency
V	volume of system, m^3
ΔV	change in V, m^3
$\Delta \ln V$	change in natural logarithm of V
v	vibrational quantum number
W	energy difference between top of potential well and rotationless ground vibrational state, m^{-1} (see fig. 8 and table III)
$W_o(\theta), W_I(\theta), W_{II}(\theta)$	integrals called W(0), W(1), and W(2), respectively, in ref. 18
w_i (i = 1, 2, 5, 6, 7)	multipliers for Δn_i in eq. (B14), $1/\text{mole}^2$
$\underline{X}$	matrix for iterative corrections, 1/mole
$\underline{X}^{-1}$	inverse of matrix for iterative corrections, moles
$\underline{Y}$	initial column vector, 1/mole
y_1	first element in $\underline{Y}$, 1/mole
Z	number of elementary charges ion (or atom) possesses after ionization
Z_c	coulomb compressibility
z_i (i=1, 2, . . ., 7)	net number of elementary charges on species i (1, 0, or -1)
α_i (i=1, 2, . . ., 7)	mass parameter for species i, $(m^3)(K^{3/2})/\text{mole}$
β	Morse parameter, m^{-1}
γ_h	contribution of a state of H_2^* to q_4' (no cutoff)
δ	term value difference between dissociation asymptotes, m^{-1} (see fig. 9)

ϵ_o	electric permittivity of free space, $C^2/N\text{-}m^2$
ζ_v	contribution of v states of $H_2^{\ddagger}$ to q'_4
η	number of gram atoms of protons, moles
η'	number of protons
θ	reduced temperature
κ	reciprocal Debye length, m^{-1}
Λ_i $(i=1,2,\ldots,7)$	characteristic volume for translation for species i, m^3
μ	reduced mass of two atoms composing a diatomic molecule, kg
μ_i $(i=1,2,\ldots,7)$	chemical potential of species i, J
ρ	density, kg/m^3
σ	symmetry number
φ_n	contribution of H with principal quantum number n to q_1 before employing cutoff
Ω_v	contribution of states with vibrational quantum number v to q'_6
ω	Morse oscillator vibrational constant, m^{-1}
ω'	fundamental vibrational frequency, m^{-1} (see fig. 8)

Subscripts:

DH	with coulomb interactions between free charged particles
d	desired value
ex	excess due to coulomb interactions between free charged particles
id	ideal gas
0	previous iteration
1	hydrogen atom, H
2	proton, H^+
3	free electron, e^-
4	hydrogen molecule, H_2
5	negative hydrogen ion, H^-
6	hydrogen diatomic molecular ion, H_2^+
7	hydrogen triatomic molecular ion, H_3^+

Superscripts:

*	electronically excited
‡	electronic ground state

Unless otherwise indicated, partial derivatives are taken with respect to one of the eight variables n_1, n_2, n_3, n_4, n_5, n_6, n_7, or V, and the other seven variables and T are understood to be held constant. The moles used in this report are gram moles.

APPENDIX B

COMPUTER PROGRAM FOR COMPONENTS OF HYDROGEN PLASMA INCLUDING MINOR SPECIES

The computer program described in this appendix computes number densities and other properties of a hydrogen plasma either with or without coulomb interactions between free charged particles. The assumptions and restrictions have already been given in the main text.

Analyses

Three analyses were used. The low-temperature analysis for temperatures from 300 to 1300 K has already been given, as has the medium-temperature analysis for temperatures from 1300 to 2000 K. Neither of these analyses required iteration.

The first part of the high-temperature analysis for temperatures from 2000 to 40 000 K has also been given (eqs. (1) to (21)). In this section these equations are put in a convenient form for iteration, and the iteration procedure is given.

Substituting equation (1) into equation (6), dividing by RT, and converting from numbers of particles to moles give

$$g \equiv \frac{G}{RT} = -\sum_{i=1}^{7} n_i \ln \frac{Vq_i}{\Lambda_i N_o n_i} - \frac{1}{8\pi N_o V^{1/2}} \left(\frac{e^2 N_o}{\epsilon_o kT} \sum_{i=1}^{7} z_i^2 n_i \right)^{3/2} \tag{B1}$$

Substituting equation (1) into equation (8), dividing by p_o, and converting from numbers of particles to moles give

$$s \equiv \frac{p}{p_o} = \frac{RT}{p_o V} \sum_{i=1}^{7} n_i - \frac{kT}{24\pi p_o} \left(\frac{e^2 N_o}{\epsilon_o kTV} \sum_{i=1}^{7} z_i^2 n_i \right)^{3/2} \tag{B2}$$

The desired value of s is p_d/p_o, which is designated s_d. Converting equation (10) from numbers of particles to moles yields

$$\eta \equiv \frac{\eta'}{N_o} = n_1 + n_2 + 2n_4 + n_5 + 2n_6 + 3n_7 \tag{B3}$$

The desired value of η can be any constant and is designated η_d. From equation (9)

$$n_3 + n_5 = n_2 + n_6 + n_7 \tag{B4}$$

During the iteration, this equality may not be met exactly, so C is defined as

$$C = n_3 + n_5 - n_2 - n_6 - n_7 \tag{B5}$$

The desired value of C is, of course, 0.

To find a minimum in g (eq. (B1)) subject to three constraints (eqs. (B2), (B3), and (B5)), all four equations are expanded in Taylor series.

$$g = g_0 + \sum_{i=1}^{7} \left(\frac{\partial g}{\partial n_i}\right)_0 \Delta n_i + \left(\frac{\partial g}{\partial V}\right)_0 \Delta V + \frac{1}{2} \sum_{i=1}^{7} \left(\frac{\partial^2 g}{\partial n_i^2}\right)_0 (\Delta n_i)^2 + \frac{1}{2}\left(\frac{\partial^2 g}{\partial V^2}\right)_0 (\Delta V)^2$$

$$+ \sum_{i=1}^{7} \left(\frac{\partial^2 g}{\partial n_i \partial V}\right)_0 \Delta n_i \, \Delta V + \sum_{i=1}^{6} \sum_{j=i+1}^{7} \left(\frac{\partial^2 g}{\partial n_i \partial n_j}\right)_0 \Delta n_i \, \Delta n_j \tag{B6}$$

In taking partial derivatives of g, q_1 and q_4 were assumed to be constants.

$$s_d = s_0 + \sum_{i=1}^{7} \left(\frac{\partial s}{\partial n_i}\right)_0 \Delta n_i + \left(\frac{\partial s}{\partial V}\right)_0 \Delta V \tag{B7}$$

$$\eta_d = \eta_0 + \sum_{i=1}^{7} \left(\frac{\partial \eta}{\partial n_i}\right)_0 \Delta n_i \tag{B8}$$

$$0 = C_0 + \sum_{i=1}^{7} \left(\frac{\partial C}{\partial n_i}\right)_0 \Delta n_i \tag{B9}$$

To simplify the nomenclature, the subscripts 0 are dropped. To avoid the 11 × 11 matrix entailed by the use of three Lagrange multipliers to find a minimum in g subject to the constraints, equations (B7) to (B9) are solved for Δn_3, Δn_4, and ΔV.

$$\Delta n_3 = -C - \Delta n_5 + \Delta n_2 + \Delta n_6 + \Delta n_7 \tag{B10}$$

$$\Delta n_4 = \frac{1}{2} (\eta_d - \eta) - \frac{1}{2} \Delta n_1 - \frac{1}{2} \Delta n_2 - \frac{1}{2} \Delta n_5 - \Delta n_6 - \frac{3}{2} \Delta n_7 \tag{B11}$$

$$\begin{aligned} \Delta V = \frac{1}{\frac{\partial s}{\partial V}} \Bigg\{ & s_d - s - \frac{\partial s}{\partial n_1} \Delta n_1 - \frac{\partial s}{\partial n_2} \Delta n_2 - \frac{\partial s}{\partial n_3} (\Delta n_2 + \Delta n_6 + \Delta n_7 - C - \Delta n_5) \\ & - \frac{\partial s}{\partial n_4} \left[\frac{1}{2} (\eta_d - \eta) - \frac{1}{2} \Delta n_1 - \frac{1}{2} \Delta n_2 - \frac{1}{2} \Delta n_5 - \Delta n_6 - \frac{3}{2} \Delta n_7\right] \\ & - \frac{\partial s}{\partial n_5} \Delta n_5 - \frac{\partial s}{\partial n_6} \Delta n_6 - \frac{\partial s}{\partial n_7} \Delta n_7 \Bigg\} \end{aligned} \tag{B12}$$

Equations (B10) to (B12) are then substituted into equation (B6). The conditions for a minimum in g are then

$$\frac{\partial g}{\partial \Delta n_i} = 0 \qquad (i = 1, 2, 5, 6, 7) \tag{B13}$$

For an i of 1, equation (B13) takes the form

$$w_1 \Delta n_1 + w_2 \Delta n_2 + w_5 \Delta n_5 + w_6 \Delta n_6 + w_7 \Delta n_7 - y_1 = 0 \tag{B14}$$

where w_1, w_2, w_5, w_6, w_7, and y_1 are complicated functions independent of Δn_1, Δn_2, Δn_5, Δn_6, and Δn_7. Equation (B14) is approximately

$$w_1n_1 \, \Delta \ln n_1 + w_2n_2 \, \Delta \ln n_2 + w_5n_5 \, \Delta \ln n_5 + w_6n_6 \, \Delta \ln n_6 + w_7n_7 \, \Delta \ln n_7 - y_1 = 0 \qquad \text{(B15)}$$

Similar equations follow for $i = 2, 5, 6$, and 7. These five equations can be written in matrix notation as

$$\underline{X}\,\underline{\mathscr{D}} - \underline{Y} = 0 \qquad \text{(B16)}$$

where $\underline{X}$ is a 5×5 matrix, $\underline{Y}$ is a five-element column vector, and

$$\begin{bmatrix} \mathscr{D}_{01} \\ \mathscr{D}_{02} \\ \mathscr{D}_{03} \\ \mathscr{D}_{04} \\ \mathscr{D}_{05} \end{bmatrix} \equiv \underline{\mathscr{D}} \equiv \begin{bmatrix} \Delta \ln n_1 \\ \Delta \ln n_2 \\ \Delta \ln n_5 \\ \Delta \ln n_6 \\ \Delta \ln n_7 \end{bmatrix} = \underline{X}^{-1}\underline{Y} \qquad \text{(B17)}$$

To find a minimum in g, initial estimates are provided for the seven n_i and V, and $\underline{\mathscr{D}}$ is found from equation (B17). From equation (B10)

$$\Delta \ln n_3 = \frac{-C - n_5 \, \Delta \ln n_5 + n_2 \, \Delta \ln n_2 + n_6 \, \Delta \ln n_6 + n_7 \, \Delta \ln n_7}{n_3} \qquad \text{(B18)}$$

From equation (B11)

$$\Delta \ln n_4 = \frac{\eta_d - \eta - n_1 \, \Delta \ln n_1 - n_2 \, \Delta \ln n_2 - n_5 \, \Delta \ln n_5 - 2n_6 \, \Delta \ln n_6 - 3n_7 \, \Delta \ln n_7}{2n_4} \qquad \text{(B19)}$$

From equation (B12) and the relations $\partial s/\partial n_1 = \partial s/\partial n_4$ and $\partial s/\partial n_2 = \partial s/\partial n_3 = \partial s/\partial n_5 = \partial s/\partial n_6 = \partial s/\partial n_7$

$$\Delta \ln V = \frac{1}{V \dfrac{\partial s}{\partial V}} \Bigg[s_d - s - \frac{1}{2} \frac{\partial s}{\partial n_1} n_1 \, \Delta \ln n_1 + \left(\frac{1}{2} \frac{\partial s}{\partial n_1} - 2 \frac{\partial s}{\partial n_2} \right) n_2 \, \Delta \ln n_2 + \frac{1}{2} \frac{\partial s}{\partial n_1} n_5 \, \Delta \ln n_5$$

$$+ \left(\frac{\partial s}{\partial n_1} - 2 \frac{\partial s}{\partial n_2} \right) n_6 \, \Delta \ln n_6 + \left(\frac{3}{2} \frac{\partial s}{\partial n_1} - 2 \frac{\partial s}{\partial n_2} \right) n_7 \, \Delta \ln n_7 + C \frac{\partial s}{\partial n_2} - \frac{1}{2} \frac{\partial s}{\partial n_1} (\eta_d - \eta) \Bigg] \qquad \text{(B20)}$$

The logarithms of the seven n_i and V are corrected by means of equations (B17) to (B20), and the next iteration may be begun.

Program Procedure

The program is in FORTRAN IV, IBM Version 13, for an IBM 7094II/7044 Direct-Coupled System with 32 000-word storage. The names of the FORTRAN variables and their corresponding symbols, equations, or comments are as follows

FORTRAN symbol	Mathematical symbol	Comments or equation
A(5, 11)	$\underline{X}^{-1}$	$\underline{X}^{-1}$ is contained in the square subarray A(1, 6) to A(5, 10)
AKAP	κ	reciprocal Debye length
AKP1	K_{p1}	equilibrium constant
AKP2		$s'_6/s'_1 s'_2$ for ideal gas
AKP4		$s'_2 s'_3/s'_1$ for ideal gas
AKP5	K_{p5}	equilibrium constant
AKP7H		$K_{p7}^{1/2}$
ALGM(7)		$\ln n_i$
ALPHA(7)	α_i	mass parameter for species i
ALV		$\ln V$
ARB1		arbitrary multiplier for r_o (always 1)
ARB2		arbitrary multiplier for ΔI (always 1)
BETA(6, 23)	β	Morse parameter (see table II for subscripts)
C	C	excess of negative charges over positive charges
CN(7)	$\hat{N}_i$	number density for species i
CNT		$\sum_{i=1}^{7} \hat{N}_i$
CN1(17)	$\hat{N}_{1n}$	number density of H with principal quantum number n

FORTRAN symbol	Mathematical symbol	Comments or equation
CN1S		$\sum_{n=2}^{17} \hat{N}_{1n}$
CN4G	$\hat{N}_4^\ddagger$	number density of $H_2^\ddagger$
CN4H(6,23)		number density of a state of H_2^* (see table II for subscripts)
CN4S		number density of H_2^* (all states)
CN4V(15)		number density of $H_2^\ddagger$ with vibrational quantum number v
CN6V(20)		number density of H_2^+ with vibrational quantum number v
CUT1		$(r_o/a_o)^{1/2}$ (approximate principal quantum number at Bethe cutoff)
CUT2		$(R_y/\Delta I)^{1/2}$ (approximate principal quantum number at Debye-Hückel cutoff)
D(5)	$\underline{\mathscr{D}}$	correction column vector
DH		0 for ideal gases; 1 for Debye-Hückel plasma (normally 1)
DELI	ΔI	absolute value of lowering of ionization potential
DELIN		new value of ΔI
DELLGM(7)		$\Delta \ln n_i$
DELLV		$\Delta \ln V$
ED(6,23)		hcD/k (see table II for subscripts)
EEXP		$e^{-u/2}$
EF(6,23)		$hc\omega'/k$ (see table II for subscripts)
EH(17)		hcT_e/k for H with principal quantum number n
EH2(6,23)		$hc\tilde{T}/k$ (see table II for subscripts)
ERETA		$\eta_d - \eta$
ERS		$s_d - s$
ETA	η	actual gram-atoms of protons

FORTRAN symbol	Mathematical symbol	Comments or equation
ETAD	η_d	desired gram-atoms of protons (always 3)
FH2(15, 39)	f	rotational term values for H_2
FH2P(20, 42)	f	rotational term values for H_2^+
FN(7)		$\partial g/\partial n_i$
FNN(7, 7)		$\partial^2 g/\partial n_i \partial n_j$
FNV(7)		$\partial^2 g/\partial V \partial n_i$
FV		$\partial g/\partial V$
FVV		$\partial^2 g/\partial V^2$
GAM(6, 23)	γ_h	contribution of a state of H_2^* to q_4' (no cutoff) (see table II for subscripts)
GAMC(6, 23)		$F_n \gamma_h$ (see table II for subscripts)
GAMCIM		$F_n \gamma_h$ with F_n calculated for Bethe cutoff
GH2(15)	G_v	vibrational term value for $H_2^{\ddagger}$
GH2P(20)	G_v	vibrational term value for H_2^+
GMO(7)	n_i	number of moles of species i
IFLAG		0 for same DH, p_d, and IPR for next case; 1 for read new DH - p_d - IPR card for next case
IMAX(23)		maximum value of first subscript of H_2^* for value of second subscript given in parentheses (see table II for subscripts)
IPR		0 for long output; 1 for short output
I1		number of iterations for cutoff to converge in high-temperature iteration (999 if no convergence or if medium- or low-temperature composition calculated)
I2		number of iterations for n_i and V to converge in high-temperature iteration (999 if no convergence; 998 if medium- or low-temperature composition calculated)
I9		index for high-temperature iterations

FORTRAN symbol	Mathematical symbol	Comments or equation
LIM		limit on I9 (always 15)
OMEGA(20)	Ω_v	contribution of states with vibrational quantum number v to q'_6
PD	p_d	desired pressure
PHI(17)	φ_n	contribution of states with principal quantum number n to q_1 (no cutoff)
PHIC(17)		first member is 2, others are $F_n \varphi_n$
PHICN		$F_n \varphi_n$ with F_n calculated for Bethe cutoff
PR		$p'_o V/RT$
PROD(7)		$N_o \Lambda_i$
PRODD		$\frac{3}{16\pi N_o} \left[\left(\frac{e^2 N_o}{\epsilon_o kT} \right)^3 \frac{1}{V} \sum_{i=1}^{7} z_i^2 n_i \right]^{1/2}$
PRODDD		$\frac{3}{32\pi N_o} \left(\frac{e^2 N_o}{\epsilon_o kTV} \right)^{3/2} \left(\sum_{i=1}^{7} z_i^2 n_i \right)^{1/2}$
PO	p_o	reference pressure for high-temperature iteration (always 10^6 N/m^2)
POP	p'_o	reference pressure for equilibrium constants (always 1.01325×10^5 N/m^2)
Q(7)	q_i	partition function for species i referred to internal energy of $H^{\ddagger}$ atoms and free electrons
QUOT		$T^{3/2}$
Q4P	q'_4	partition function of H_2 referred to rotationless ground vibrational state of $H_2^{\ddagger}$
Q6P	q'_6	partition function of H_2^+ referred to rotationless ground vibrational state
Q7P	q'_7	partition function of H_3^+ referred to rotationless ground vibrational state

FORTRAN symbol	Mathematical symbol	Comments or equation
Q7PT(67)		table of q_7' having one-to-one correspondence with TT table
R	r_c	ratio of equivalent concentration to critical equivalent concentration
RAT	R_h	vibrational quantum correction
RAT1		absolute value of relative change in r_o in one iteration
RAT2		absolute value of relative change in ΔI in one iteration
RE(6,23)	r_e	equilibrium internuclear distance (see table II for subscripts)
REL(8)		absolute value of relative change in n_i and V in one iteration
RES		$\frac{3}{32\pi N_o}\left(\frac{e^2 N_o}{\epsilon_o kT}\right)^{3/2}\left(V\sum_{i=1}^{7} z_i^2 n_i\right)^{-1/2}$
RHO	ρ	density
RO	r_o	half the average distance between neighboring molecules
RON		new value for r_o
ROOT		$\left(\frac{10^{-16} e^2 N_o}{\epsilon_o kTV}\sum_{i=1}^{7} z_i^2 n_i\right)^{1/2}$
ROOT1		negative of average of two adjacent ROOTA in Rydberg series
ROOT2		negative of average of two adjacent ROOTA in Rydberg series
ROOTA(18)		$a_n^{1/2}$ for H
ROOTA(7,23)		$a_n^{1/2}$ for H_2^* (see table II for subscripts)
ROOTR		$(r_o\text{ARB1})^{1/2}$

FORTRAN symbol	Mathematical symbol	Comments or equation
S		p/p_o
SD		p_d/p_o
SIGMA1		$\sum_{\text{odd } J} (2J + 1)\exp\left(- \frac{hcf}{kT}\right)$ for $H_2^\ddagger$
SIGMA2		$\sum_{\text{even } J} (2J + 1)\exp\left(- \frac{hcf}{kT}\right)$ for $H_2^\ddagger$
SIGMA3		$\sum_{\text{odd } K} (2K + 1)\exp\left(- \frac{hcf}{kT}\right)$ for H_2^+
SIGMA4		$\sum_{\text{even } K} (2K + 1)\exp\left(- \frac{hcf}{kT}\right)$ for H_2^+
SM		$\sum_{i=1}^{7} z_i^2 n_i$
SN(2)		$\partial s/\partial n_i$ where i is 1 or 2
SN1SV		$(\partial s/\partial n_1)/(\partial s/\partial V)$
SN2SV		$(\partial s/\partial n_2)/(\partial s/\partial V)$
SP(7)		p_i/p'_o
SPD		p_d/p'_o
SP3		$(K_{p4}p_1/p'_o)^{1/2}$
STAR1		average of two adjacent I in Rydberg series
STAR2		average of two adjacent I in Rydberg series
STARI(7,23)	I	for H_2^* (see table II for subscripts)
STARI(18)	I	for H with principal quantum number n
SUM	$q'_{H_2^\ddagger}$	contribution of $H_2^\ddagger$ to q'_4
SUMM		$\sum_{i=1}^{7} n_i$
SUM1		$\sum_{n=2}^{17} F_n\varphi_n$

FORTRAN symbol	Mathematical symbol	Comments or equation
SUM4		$\sum F_n\gamma_h$
SUM9		$\hat{N}_2 + \hat{N}_3 + \hat{N}_5 + \hat{N}_6 + \hat{N}_7$
SV		$\partial s/\partial V$
T	T	temperature
THETA	θ	reduced temperature
THETAT(29)		table of θ having one-to-one correspondence with W0T, W1T, and W2T tables
TOL1		maximum allowable absolute value of relative change in r_o and ΔI in last iteration before freezing cutoffs (always 0.001)
TOL2		maximum allowable absolute value of relative change in n_i and V for last iteration (always 0.00001)
TS1		dividing point of low and medium temperatures
TS2		dividing point of medium and high temperatures
TT(67)		table of T having one-to-one correspondence with Q7PT table
U	u	dimensionless fundamental vibration frequency
V	V	volume of system
W		$\dfrac{s_d - s + C\dfrac{\partial s}{\partial n_2} - \dfrac{1}{2}\dfrac{\partial s}{\partial n_1}(\eta_d - \eta)}{\dfrac{\partial s}{\partial V}}$
WEIGHT(6,23)	g_e	electronic statistical weight (see table II for subscripts)
WO	W_o	integral called W(0) in ref. 18
WOT(29)		table of W_o having one-to-one correspondence with θ table
W1	W_I	integral called W(1) in ref. 18

FORTRAN symbol	Mathematical symbol	Comments or equation
W1T(29)		table of W_I having one-to-one correspondence with θ table
W2	W_{II}	integral called W(2) in ref. 18
W2T(29)		table of W_{II} having one-to-one correspondence with θ table
X(5, 5)	$\underline{X}$	matrix for iterative corrections
Y(5)	$\underline{Y}$	initial column vector
Z(7)		z_i^2
ZC	Z_c	coulomb compressibility
ZETA(15)	ζ_v	contribution of v states of $H_2^\ddagger$ to q_4'

(Units are given in appendix A.)

A simplified flow diagram of the program is shown in figure 6. The input quantity DH determines whether or not coulomb interactions between free charged particles are included. Other features of the flow diagram are discussed in the following paragraphs.

Two sets of criteria were used for convergence because q_1 and q_4 were assumed to be constants when taking partial derivatives of g. Actually, q_1 and q_4 depend on the n_i because of the cutoffs, but this dependence must be neglected when taking partial derivatives if the solutions are to obey Saha's equations (ref. 34) as is customary. This results in an inconsistency. Problems due to the inconsistency were averted by using two sets of criteria for convergence, as shown in figure 6. The first set was that relative changes in one iteration in both r_o and ΔI must be less than TOL1 (set at 0.001). After these criteria were met, r_o and ΔI and, hence, the cutoffs were not changed again. The second set of criteria was that relative changes in the seven n_i and V be less than TOL2 (set at 0.00001).

There are two options for output. If the input quantity IPR is 0, the long output (1 page per case) is used. If IPR is not 0 and the iteration (in the case of high temperature) converges, the short output (1 line per case) is used.

A block diagram of the program and the eight subprograms is given in figure 7.

Sample Problems

An input form with data for seven sample cases is given in table VI. Note that

IFLAG is 1 on the second card because it is desired to change IPR by means of the next card. The output is shown in table VII. Case 1 had long output, whereas cases 2 to 7 had short output. The order of the quantities in short output is T and number densities for $H_2^\ddagger$, H_2^*, $H^\ddagger$, H^*, e^-, H^-, H_3^+, H_2^+, H^+, H_2, and H.

Running Characteristics

A control card is required so that minor underflows are not printed out. With short output 168 cases required 1.56 minutes to execute. With long output 45 cases required 0.71 minute to execute. For all high-temperature problems, I1 was between 2 and 4, whereas I2 was between 3 and 8.

Listing of Program

```
$IBFTC MAIN    DEBUG
C PROGRAM FOR COMPONENTS OF A HYDROGEN PLASMA INCLUDING MINOR SPECIES
C
      DIMENSION IMAX(23),GAM(6,23),GAMC(6,23),PHI(17),PHIC(17),Q(7),
     1PROD(7),ALPHA(7),EH(17),EF(6,23),ED(6,23),EH2(6,23),WEIGHT(6,23),
     2RE(6,23),BETA(6,23),JP1M(15),KP1M(20),CN(7),GH2(15),GH2P(20),
     3FH2(15,39),FH2P(20,42),Q7PT(67),TT(67),THETAT(29),WOT(29),W1T(29),
     4W2T(29),ZETA(15),Z(7),CN1(17),CN4H(6,23),CN4V(15),CN6V(20),
     5OMEGA(20),REL(8),SP(7)
      COMMON/BLOCK1/DH,T,PO,PROD,ETAD,SD/BLOCK2/PHI,PHIC,SUM1/BLOCK3/SUM
     1,GAM,GAMC,SUM4/BLOCK4/IMAX/BLOCK5/ARB1,ARB2/BLOCK6/Z
     2/BLOCK7/ALPHA,EH,EF,ED,EH2,WEIGHT,RE,BETA,JP1M,KP1M,GH2,GH2P,FH2/
     3BLOCK8/FH2P,Q7PT,TT,THETAT,WOT,W1T,W2T
      DOUBLE PRECISION V,GMO(7),X(5,5),Y(5),S,ETA,C,SM,ROOT,SUMM,A(5,11)
     1,SN(2),SV,D(5),DELLGM(7),DELLV,ALGM(7),ALV
    2 READ(5,200) DH,PD,IPR
      WRITE(6,201)DH,PD,IPR
C ASSIGN VALUES TO CONSTANTS.
      TS1=1300.
      TS2=2000.
      PO=1.E+6
      POP=1.01325E+5
      TOL1=.001
      TOL2=.00001
      ARB1=1.
      ARB2=1.
      LIM=15
      ETAD=3.
      K=0
    1 READ(5,202) T,IFLAG
C END OF INPUT. FIND CONTRIBUTION OF GROUND ELECTRONIC STATE OF H2 TO H2
C PARTITICN FUNCTION.
      SUM=0.
      DO 3 KVP1=1,15
      SIGMA1=0.
      MAX=JP1M(KVP1)
      DO 4 JP1=2,MAX,2
    4 SIGMA1=SIGMA1+FLOAT(2*JP1-1)*EXPC(-.0143879*FH2(KVP1,JP1)/T)
      SIGMA2=0.
      DO 5 JJP1=1,MAX,2
    5 SIGMA2=SIGMA2+FLOAT(2*JJP1-1)*EXPC(-.0143879*FH2(KVP1,JJP1)/T)
      ZETA(KVP1)=.25*EXPC(-.0143879*GH2(KVP1)/T)*(3.*SIGMA1+SIGMA2)
      DEBUG SIGMA1,SIGMA2,ZETA(KVP1)
    3 SUM=SUM+ZETA(KVP1)
C INITIALIZE VARIABLES.
      RO=1.E-8*(3.2958*T/PD)**.33333
```

```
      DEBUG RO,SUM
      RON=RO
      DELI=0.
      DO 46 NI=1,7
   46 DELLGM(NI)=0.
      DELLV=0.
      ERS=0.
      C=0.
      ERETA=0.
      Q6P=0.
      I1=999
      I2=998
C TEST IF T IS LOW.
      IF(T-TS1)7,7,8
C FIND LOW T COMPOSITION FROM HERE UP TO STATEMENT 8.
    7 Q(1)=2.
      CN1(1)=SQRT(PD*SQRT(T)/(1.0775E-3*SUM))*Q(1)*(1.E+23*EXP(-25980.0
     1/T))/1.3805
      CN1S=0.
      CN(2)=0.
      CN(3)=0.
      CN(4)=PD/(1.3805E-23*T)
      CN4S=0.
      CN(5)=0.
      CN(6)=0.
      CN(7)=0.
      CN4G=CN(4)
      CN(1)=CN1(1)
      Q4P=SUM
      Q7P=0.
      GO TO 100
C FOR MEDIUM AND HIGH T FIND CONTRIBUTIONS OF H2* TO H2 PARTITION
C FUNCTION ASSUMING NO CUTOFF.
    8 DO 6 M=1,23
      IMA=IMAX(M)
      DO 6 II=2,IMA
      U=EF(II,M)/T
      EEXP=EXP(-U/2.)
      RAT=U*EEXP/(1.-EEXP**2)
      THETA=T/ED(II,M)
      W0=BINT(THETAT,W0T,THETA,29)
      W1=BINT(THETAT,W1T,THETA,29)
      W2=BINT(THETAT,W2T,THETA,29)
      GAM(II,M)=4.7660*WEIGHT(II,M)*EXPC(-EH2(II,M)/T)*T**1.5*(1.E+26*
     1RE(II,M)**2*W0/BETA(II,M)+2.E+26*RE(II,M)*W1/BETA(II,M)**2+1.E+26
     2*W2/BETA(II,M)**3)*RAT
      DEBUG U,RAT,THETA,W0,W1,W2,GAM(II,M),II,M
    6 CONTINUE
C FIND CONTRIBUTIONS OF ELECTRONIC STATES OF H TO H PARTITION FUNCTION
C ASSUMING NO CUTOFF.
      DO 9 N=1,17
    9 PHI(N)=FLOAT(2*N**2)*EXPC(-EH(N)/T)
      DEBUG (PHI(I),I=1,17)
C FIND PARTITION FUNCTIONS OF H AND H2 WITH CUTOFF.
      Q(1)=Q1PF(RO,DELI)
      DEBUG (PHIC(I),I=1,17)
```

```
      Q4P=Q4PF(RO,DELI)
C FIND PARTITION FUNCTION OF H3+.
      Q7P=BINT(TT,Q7PT,T,67)
C FIND EQUILIBRIUM CONSTANTS USED FOR MEDIUM AND HIGH T.
      AKP1=1.0775E-3*Q4P*POP*EXP(51959.9/T)/(Q(1)**2*T**2.5)
      AKP5=15.010*POP*EXP(8947.4/T)/(Q(1)*T**2.5)
      AKP7H=SQRT(1.4211E-3*Q7P)*T**.625*EXP(-65567./T)/(Q4P**.75*POP**
     1.25)
      SPD=PD/POP
      DEBUG Q(1),Q4P,Q7P,AKP1,AKP5,AKP7H,SPD,((GAMC(I,L),I=2,6),L=1,23)
C TEST IF T IS MEDIUM OR HIGH.
      IF(T-TS2)10,10,13
C FIND MEDIUM T COMPOSITION FROM HERE THROUGH STATEMENT 11.
   10 SP(1)=(SQRT(4.*SPD*AKP1+1.)-1.)/(2.*AKP1)
      SP(4)=SPD-SP(1)
      SP(3)=AKP7H*SQRT(SP(4)**1.5/(AKP5*SP(1)+1.))
      SP(7)=AKP7H*SP(4)**.75*SQRT(AKP5*SP(1)+1.)
      SP(5)=SP(7)-SP(3)
      SP(2)=0.
      SP(6)=0.
      DO 11 NA=1,7
   11 CN(NA)=SP(NA)*POP/(1.3805E-23*T)
C FIND QUANTITIES NEEDED FOR MEDIUM AND HIGH T.
   12 CN1S=SUM1*CN(1)/Q(1)
      CN1(1)=CN(1)-CN1S
      CN4S=SUM4*CN(4)/Q4P
      CN4G=CN(4)-CN4S
  100 DELIN=.11614E-2*SQRT(.20998E-3*(CN(2)+CN(3)+CN(5)+CN(6)+CN(7))/T)
      GO TO 40
C FIND HIGH T COMPOSITION FROM HERE UP TO STATEMENT 40.
   13 SD=PD/PO
      I2=999
C FIND H2+ PARTITION FUNCTION.
      DO 14 KKVP1=1,20
      SIGMA3=0.
      MAX=KP1M(KKVP1)
      DO 15 KP1=2,MAX,2
   15 SIGMA3=SIGMA3+FLOAT(2*KP1-1)*EXPC(-.0143879*FH2P(KKVP1,KP1)/T)
      SIGMA4=0.
      DO 16 KKP1=1,MAX,2
   16 SIGMA4=SIGMA4+FLOAT(2*KKP1-1)*EXPC(-.0143879*FH2P(KKVP1,KKP1)/T)
      OMEGA(KKVP1)=EXPC(-.0143879*GH2P(KKVP1)/T)*(1.5*SIGMA3+.5*SIGMA4)
      DEBUG SIGMA3,SIGMA4,OMEGA(KKVP1)
   14 Q6P=Q6P+OMEGA(KKVP1)
C FIND PARTITION FUNCTIONS REFERRED TO H AND E-.
      Q(2)=EXP(-157805./T)
      Q(3)=2.
      Q(4)=Q4P*EXP(51959.9/T)
      Q(5)=EXP(8947.4/T)
      Q(6)=Q6P*EXP(-127044./T)
      Q(7)=Q7P*EXP(-53195./T)
C FIND EQUILIBRIUM CONSTANTS USED FOR INITIAL ESTIMATES FOR HIGH T.
      AKP2=.0010779*Q6P*POP*EXP(30760.5/T)/(Q(1)*T**2.5)
      AKP4=.066618*T**2.5*EXP(-157805./T)/(Q(1)*POP)
      DEBUG SD,Q6P,AKP2,AKP4,(Q(I),I=1,7)
C MAKE INITIAL ESTIMATES FOR HIGH T.
```

```
      SP(1)=(DSQRT(1.D0+4.D0*AKP1*(2.D0*(AKP4-DSQRT(AKP4)*DSQRT(AKP4+
     1SPD))+SPD))-1.D0)/(2.D0*AKP1)
      SP(4)=AKP1*SP(1)**2
      SP(3)=AKP7H*SQRT(SP(4)**1.5/(AKP5*SP(1)+1.))
      SP3=SQRT(AKP4*SP(1))
      DEBUG SP(1),SP(3),SP(4),SP3
      IF(SP(3)-SP3)18,18,17
   17 SP(7)=AKP7H*SP(4)**.75*SQRT(AKP5*SP(1)+1.)
      SP(5)=SP(7)-SP(3)
      SP(2)=SP(1)*AKP4/SP(3)
      GO TO 119
   18 SP(3)=SP3
      SP(2)=SP3
      SP(7)=AKP7H**2*SP(4)**1.5/SP(3)
      SP(5)=AKP5*SP(1)*SP(3)
  119 SP(6)=SP(1)*SP(2)*AKP2
      V=8.3143*T*ETAD/(POP*(SP(1)+SP(2)+2.*SP(4)))
      PR=POP*V/(8.3143*T)
      DO 19 NB=1,7
      GMO(NB)=PR*SP(NB)
   19 ALGM(NB)=DLOG(GMO(NB))
      ALV=DLOG(V)
      SM=0.
      QUOT=T**1.5
      DO 20 JJ=1,7
      PROD(JJ)=ALPHA(JJ)/QUOT
   20 SM=SM+Z(JJ)*GMO(JJ)
      ROOT=DSQRT(1.2646D4*SM/(T*V))
      DEBUG V,PR,ALV,SM,ROOT,(GMO(I),ALGM(I),I=1,7)
C ENTER HIGH T ITERATION EXTENDING THROUGH STATEMENT 122.
      DO 122 I9=1,LIM
      SUMM=0.
      DO 21 NC=1,7
   21 SUMM=SUMM+GMO(NC)
      S= 8.3143*T*SUMM/(PO*V)-.18310*T*ROOT**3*DH/PO
      ETA=GMO(1)+GMO(2)+2.*GMO(4)+GMO(5)+2.*GMO(6)+3.*GMO(7)
      C=GMO(3)+GMO(5)-GMO(2)-GMO(6)-GMO(7)
      DEBUG SUMM,S,ETA,C
C FIND MATRIX AND INITIAL VECTOR FOR ITERATIVE CORRECTIONS.
      CALL MATR(V,GMO,S,ETA,C,Q,ROOT,SUMM,SM,X,Y,SN,SV)
C INVERT MATRIX.
      CALL INVERT(X,A)
      DEBUG ((A(I,L),L=6,10),I=1,5)
C FIND CORRECTION VECTOR FOR ITERATIVE CORRECTIONS.
  199 DO 23 ND=1,5
      D(ND)=0.
      DO 23 NE=1,5
   23 D(ND)=D(ND)+A(ND,NE+5)*Y(NE)
      DELLGM(1)=D(1)
      DELLGM(2)=D(2)
      DELLGM(5)=D(3)
      DELLGM(6)=D(4)
      DELLGM(7)=D(5)
      DELLGM(3)=(-C-GMO(5)*DELLGM(5)+GMO(2)*DELLGM(2)+GMO(6)*DELLGM(6)+
     1GMO(7)*DELLGM(7))/GMO(3)
      DELLGM(4)=(ETAD-ETA-GMO(1)*DELLGM(1)-GMO(2)*DELLGM(2)-GMO(5)*
```

```
     1DELLGM(5)-2.*GMO(6)*DELLGM(6)-3.*GMO(7)*DELLGM(7))/(2.*GMO(4))
      DELLV=(SD-S-.5D0*SN(1)*GMO(1)*DELLGM(1)+(.5D0*SN(1)-2.*SN(2))*
     1GMO(2)*DELLGM(2)+.5D0*SN(1)*GMO(5)*DELLGM(5)+(SN(1)-2.*SN(2))*
     2GMO(6)*DELLGM(6)+(1.5D0*SN(1)-2.*SN(2))*GMO(7)*DELLGM(7)+C*SN(2)-
     3.5D0*SN(1)*(ETAD-ETA))/(V*SV)
      DEBUG DELLV,(DELLGM(I),I=1,7)
      DO 24 NF=1,7
C MAKE ITERATIVE CORRECTIONS.
      ALGM(NF)=ALGM(NF)+DELLGM(NF)
   24 GMO(NF)=DEXP(ALGM(NF))
      ALV=ALV+DELLV
      V=DEXP(ALV)
      SM=0.
      DO 25 JJJ=1,7
   25 SM=SM+Z(JJJ)*GMO(JJJ)
      ROOT=DSQRT(1.2646D4*SM/(T*V))
      DEBUG SM,ROOT,ALV,V,(GMO(I),ALGM(I),I=1,7)
C TEST IF RO AND DELI HAVE PREVIOUSLY CONVERGED.
      IF(I1-999)27,26,27
C FIND NEW VALUES FOR RO AND DELI.
   26 RON=1.E-8*(.39640*V/(GMO(1)+GMO(2)+GMO(4)+GMO(5)+GMO(6)+GMO(7)))*
     1*.33333
      DELIN=1.1614E+5*ROOT
      RAT1=ABS((RON-RO)/RON)
      RAT2=ABS((DELIN-DELI)/DELIN)
C TEST IF RO AND DELI HAVE CONVERGED.
      IF(RAT1.LT.TOL1.AND.RAT2.LT.TOL1)I1=I9
C MAKE CORRECTIONS BASED ON NEW VALUES OF RO AND DELI.
      RO=RON
      DELI=DELIN
      Q(1)=Q1PF(RO,DELI)
      DEBUG I1,RAT1,RAT2,RO,DELI,Q(1),(PHIC(I),I=1,17)
      Q4P=Q4PF(RO,DELI)
      Q(4)=Q4P*EXP(51959.9/T)
      DEBUG Q4P,Q(4),((GAMC(I,L),I=2,6),L=1,23)
      GO TO 122
C RO AND DELI HAVING CONVERGED, FIND RELATIVE CHANGES IN MOLES AND
C VOLUME.
   27 DO 30 NG=1,7
   30 REL(NG)=DABS(DEXP(DELLGM(NG))-1.)
      REL(8)=DABS(DEXP(DELLV)-1.)
      DEBUG (REL(I),I=1,8)
C TEST IF MOLES AND VOLUME HAVE CONVERGED.
      IF(REL(1).LT.TOL2.AND.REL(2).LT.TOL2.AND.REL(3).LT.TOL2.AND
     1.REL(4).LT.TOL2.AND.REL(5).LT.TOL2.AND.REL(6).LT.TOL2.AND.
     2REL(7).LT.TOL2.AND.REL(8).LT.TOL2)GO TO 39
  122 CONTINUE
      GO TO 97
   39 I2=I9
   97 ERS=SD-S
      ERETA=ETAD-ETA
C FIND HIGH T NUMBER DENSITIES FROM MOLES AND VOLUME.
      DO 42 NH=1,7
   42 CN(NH)=6.0225E+23*(GMO(NH)/V)
      RON=1.E-8*(.39640*V/(GMO(1)+GMO(2)+GMO(4)+GMO(5)+GMO(6)+GMO(7)))*
     1*.33333
```

```
      GO TO 12
C TEST IF SHORT OUTPUT TO BE USED.
   40 IF(IPR.NE.0.AND.I2.NE.999)GO TO 43
C TEST QUANTITIES PECULIAR TO LONG OUTPUT.
      CUT1=SQRT(RO/5.2917E-11)
      IF(DELI)89,89,90
   89 CUT2=1.E+37
      GO TO 91
   90 CUT2=SQRT(10969308./DELI)
   91 SUM9=CN(2)+CN(3)+CN(5)+CN(6)+CN(7)
      CNT=SUM9+CN(1)+CN(4)
      DO 93 KVVP1=1,15
   93 CN4V(KVVP1)=CN4G*ZETA(KVVP1)/SUM
      DO 94 KKVVP1=1,20
      IF(T-TS2)102,102,101
  101 CN6V(KKVVP1)=CN(6)*OMEGA(KKVVP1)/Q6P
      GO TO 94
  102 CN6V(KKVVP1)=0.
   94 CONTINUE
      DO 95 MMM=1,23
      IW=IMAX(MMM)
      DO 95 III=2,IW
      IF(T-TS1)104,104,103
  103 CN4H(III,MMM)=CN(4)*GAMC(III,MMM)/Q4P
      GO TO 95
  104 CN4H(III,MMM)=0.
   95 CONTINUE
      DO 96 NK=2,17
      IF(T-TS1)106,106,105
  105 CN1(NK)=PHIC(NK)*CN(1)/Q(1)
      GO TO 96
  106 CN1(NK)=0.
   96 CONTINUE
      RHO=1.6734E-27*CN(1)+1.6725E-27*CN(2)+9.1091E-31*CN(3)+3.3469E-27
     1*CN(4)+1.6743E-27*CN(5)+3.3460E-27*CN(6)+5.0194E-27*CN(7)
      ZC=PD/(T*1.3805E-23*CNT)
      AKAP=SQRT(.20998E-3*SUM9/T)
      IF(T-TS1)151,151,150
  151 R=0.
      GO TO 152
  150 R=AKAP**2/(4.*(3.1416*SUM9)**.66667)
C WRITE LONG OUTPUT.
  152 WRITE(6,204)PD,T,RHO,CNT
      WRITE(6,205)ZC,AKAP,R
      WRITE(6,206)(CN(I),I=1,7)
      WRITE(6,207)(CN4V(I),I=1,15)
      WRITE(6,208) CN4G,(CN4H(I,1),I=2,4)
      WRITE(6,209)(CN4H(I,2),I=2,4)
      WRITE(6,210)(CN4H(I,3),I=2,4)
      WRITE(6,211)(CN4H(I,4),I=2,3)
      WRITE(6,212)(CN4H(I,5),I=2,3)
      WRITE(6,213)(CN4H(I,6),I=2,3)
      WRITE(6,214)(CN4H(2,I),I=7,10)
      WRITE(6,215)(CN4H(I,11),I=2,4)
      WRITE(6,216)(CN4H(I,12),I=2,3)
      WRITE(6,217)(CN4H(I,13),I=2,4)
```

```
      WRITE(6,218)(CN4H(I,14),I=2,3)
      WRITE(6,219)(CN4H(I,15),I=2,3)
      WRITE(6,220)(CN4H(I,16),I=2,3)
      WRITE(6,221)(CN4H(2,I),I=17,20)
      WRITE(6,222)((CN4H(I,L),I=2,6),L=21,22)
      WRITE(6,223)(CN4H(I,23),I=2,4)
      WRITE(6,224) CN4S
      WRITE(6,225)(CN1(I),I=1,17)
      WRITE(6,226) CN1S
      WRITE(6,227)(CN6V(I),I=1,20)
      WRITE(6,228) DELI,DELIN,RO,RON
      WRITE(6,229) CUT1,CUT2,Q(1),Q4P
      WRITE(6,230) Q6P,Q7P,ERETA,C
      WRITE(6,231) ERS,DELLV,(DELLGM(I),I=1,7)
      WRITE(6,232) ETAD,I1,I2
      IF(IFLAG)2,1,2
C CONTROL LINE SPACING ON SHORT OUTPUT.
   43 K=K+1
      IF(K-6)45,44,45
   44 K=1
      WRITE(6,262)
   45 IT=IFIX(T)
C WRITE SHORT OUTPUT.
      WRITE(6,233)IT,CN4G,CN4S,CN1(1),CN1S,CN(3),CN(5),CN(7),CN(6),CN(2)
     1,CN(4),CN(1)
C TEST IF NEW DH, PD, IPR CARD TO BE READ.
   41 IF(IFLAG)107,1,107
  107 WRITE(6,261)
      GO TO 2
  200 FORMAT(F10.0,E15.5,I5)
  201 FORMAT(1H0,3HDH ,1PE11.4,4X,3HPD ,E11.4,4X,4HIPR ,I2/1H1)
  202 FORMAT(F10.0,I5)
  204 FORMAT(1H0,9HPRESSURE ,1PE11.4,17H N/M**2    TEMP. ,E11.4,14H K
     1 DENSITY ,E11.4,33H KG/M**3    TOTAL NUMBER DENSITY ,E11.4,7H 1/M*
     2*3)
  205 FORMAT(1H ,24HCOULOMB COMPRESSIBILITY ,F8.5,28H    RECIPROCAL DEBY
     1E LENGTH ,1PE11.4,43H 1/M    EQUIV. CONC./CRITICAL EQUIV. CONC. ,
     2E11.4)
  206 FORMAT(1H0,45HSPECIES NUMBER DENSITY, PARTICLES/CUBIC METER/1X,3H
     1H ,1PE11.4,4X,3HH+ ,E11.4,4X,2HE ,E11.4,4X,3HH2 ,E11.4,4X,3HH- ,
     2E11.4,4X,4HH2+ ,E11.4,4X,4HH3+ ,E11.4)
  207 FORMAT(1H0,53HDETAILED NUMBER DENSITY FOR H2, MOLECULES/CUBIC METE
     1R/1X,67H GROUND ELECTRONIC STATE WITH VIBRATIONAL QUANTUM NUMBER O
     2F   V=0  ,1PE11.4,4X,5HV=1  ,E11.4,4X,5HV=2  ,E11.4/1X,7H  V=3  ,
     3E11.4,4X,5HV=4  ,E11.4,4X,5HV=5  ,E11.4,4X,5HV=6  ,E11.4,4X,5HV=7
     4 ,E11.4,4X,5HV=8  ,E11.4/1X,7H  V=9  ,E11.4,4X,5HV=10 ,E11.4,4X,5H
     5V=11 ,E11.4,4X,5HV=12 ,E11.4,4X,5HV=13 ,E11.4,4X,5HV=14 ,E11.4)
  208 FORMAT(1H ,31H 1SNS SINGLET SIGMA STATES WITH,11X,5HN=1  ,1PE11.4,
     14X,5HN=2  ,E11.4,4X,5HN=3  ,E11.4,4X,5HN=4  ,E11.4)
  209 FORMAT(1H ,31H 1SNP SINGLET SIGMA STATES WITH,11X,5HN=2  ,1PE11.4,
     14X,5HN=3  ,E11.4,4X,5HN=4  ,E11.4)
  210 FORMAT(1H ,28H 1SNP SINGLET PI STATES WITH,14X,5HN=2  ,1PE11.4,4X,
     15HN=3  ,E11.4,4X,5HN=4  ,E11.4)
  211 FORMAT(1H ,31H 1SND SINGLET SIGMA STATES WITH,11X,5HN=3  ,1PE11.4,
     14X,5HN=4  ,E11.4)
  212 FORMAT(1H ,28H 1SND SINGLET PI STATES WITH,14X,5HN=3  ,1PE11.4,4X,
```

```
   15HN=4   ,E11.4)
213 FORMAT(1H ,31H 1SND SINGLET DELTA STATES WITH,11X,5HN=3   ,1PE11.4,
   14X,5HN=4   ,E11.4)
214 FORMAT(1H ,25H 1S4F SINGLET SIGMA STATE,22X,1PE11.4/1X,22H 1S4F SI
   1NGLET PI STATE,25X,1PE11.4/1X,25H 1S4F SINGLET DELTA STATE,22X,1PE
   211.4/1X,23H 1S4F SINGLET PHI STATE,24X,E11.4)
215 FORMAT(1H ,31H 1SNS TRIPLET SIGMA STATES WITH,11X,5HN=2   ,1PE11.4,
   14X,5HN=3   ,E11.4,4X,5HN=4   ,E11.4)
216 FORMAT(1H ,31H 1SNP TRIPLET SIGMA STATES WITH,11X,5HN=3   ,1PE11.4,
   14X,5HN=4   ,E11.4)
217 FORMAT(1H ,28H 1SNP TRIPLET PI STATES WITH,14X,5HN=2   ,1PE11.4,4X,
   15HN=3   ,E11.4,4X,5HN=4   ,E11.4)
218 FORMAT(1H ,31H 1SND TRIPLET SIGMA STATES WITH,11X,5HN=3   ,1PE11.4,
   14X,5HN=4   ,E11.4)
219 FORMAT(1H ,28H 1SND TRIPLET PI STATES WITH,14X,5HN=3   ,1PE11.4,4X,
   15HN=4   ,E11.4)
220 FORMAT(1H ,31H 1SND TRIPLET DELTA STATES WITH,11X,5HN=3   ,1PE11.4,
   14X,5HN=4   ,E11.4)
221 FORMAT(1H ,25H 1S4F TRIPLET SIGMA STATE,22X,1PE11.4/1X,22H 1S4F TR
   1IPLET PI STATE,25X,1PE11.4/1X,25H 1S4F TRIPLET DELTA STATE,22X,1PE
   211.4/1X,23H 1S4F TRIPLET PHI STATE,24X,E11.4)
222 FORMAT(1H ,20H ALL 1SN STATES WITH,22X,5HN=5   ,1PE11.4,4X,5HN=6   ,
   1E11.4,4X,5HN=7   ,E11.4,4X,5HN=8   ,E11.4/1X,7H   N=9   ,E11.4,4X,5HN=
   210  ,E11.4,4X,5HN=11 ,E11.4,4X,5HN=12 ,E11.4,4X,5HN=13 ,E11.4,4X,
   35HN=14 ,E11.4)
223 FORMAT(1H ,7H   N=15 ,1PE11.4,4X,5HN=16 ,E11.4,4X,5HN=17 ,E11.4)
224 FORMAT(1H ,35H TOTAL IN EXCITED ELECTRONIC STATES,12X,1PE11.4)
225 FORMAT(1H0,48HDETAILED NUMBER DENSITY FOR H, ATOMS/CUBIC METER/1X,
   147H STATES WITH PRINCIPAL QUANTUM NUMBER OF   N=1   ,1PE11.4,4X,5HN=
   22   ,E11.4,4X,5HN=3   ,E11.4,4X,5HN=4   ,E11.4/1X,7H   N=5   ,E11.4,4X,
   35HN=6   ,E11.4,4X,5HN=7   ,E11.4,4X,5HN=8   ,E11.4,4X,5HN=9   ,E11.4,
   44X,5HN=10 ,E11.4/1X,7H   N=11 ,E11.4,4X,5HN=12 ,E11.4,4X,5HN=13 ,
   5E11.4,4X,5HN=14 ,E11.4,4X,5HN=15 ,E11.4,4X,5HN=16 ,E11.4/1X,7H   N=
   617 ,E11.4)
226 FORMAT(1H ,35H TOTAL IN EXCITED ELECTRONIC STATES,12X,1PE11.4)
227 FORMAT(1H0,49HDETAILED NUMBER DENSITY FOR H2+, IONS/CUBIC METER/1X
   1,67H GROUND ELECTRONIC STATE WITH VIBRATIONAL QUANTUM NUMBER OF
   2V=0   ,1PE11.4,4X,5HV=1   ,E11.4,4X,5HV=2   ,E11.4/1X,7H   V=3   ,E11.4
   3,4X,5HV=4   ,E11.4,4X,5HV=5   ,E11.4,4X,5HV=6   ,E11.4,4X,5HV=7   ,
   4E11.4,4X,5HV=8   ,E11.4/1X,7H   V=9   ,E11.4,4X,5HV=10 ,E11.4,4X,5HV=
   511 ,E11.4,4X,5HV=12 ,E11.4,4X,5HV=13 ,E11.4,4X,5HV=14 ,E11.4/1X,
   67H   V=15   ,E11.4,4X,5HV=16 ,E11.4,4X,5HV=17 ,E11.4,4X,5HV=18 ,
   7E11.4,4X,5HV=19 ,E11.4)
228 FORMAT(1H0,24HMISCELLANEOUS QUANTITIES/1X,10H DELI      ,1PE11.4,
   18X,9HDELIN     ,E11.4,8X,9HRO        ,E11.4,8X,9HRON       ,E11.4)
229 FORMAT(1H ,10H CUT1      ,1PE11.4,8X,9HCUT2      ,E11.4,8X,9HQ(1)
   1  ,E11.4,8X,9HQ4P       ,E11.4)
230 FORMAT(1H ,10H Q6P       ,1PE11.4,8X,9HQ7P       ,E11.4,8X,9HERETA
   1  ,E11.4,8X,9HC         ,D11.4)
231 FORMAT(1H ,10H ERS       ,1PE11.4,8X,9HDELLV     ,D11.4,8X,9HDELLGM(
   11),D11.4,8X,9HDELLGM(2),D11.4/1X,10H DELLGM(3),D11.4,8X,9HDELLGM(4
   2),D11.4,8X,9HDELLGM(5),D11.4,8X,9HDELLGM(6),D11.4/1X,10H DELLGM(7)
   3,D11.4)
232 FORMAT(1H+,29X,9HETAD      ,1PE11.4,8X,9HI1        ,I3,16X,9HI2
   1  ,I3/1H1)
233 FORMAT(1H ,I5,2X,1P11E11.3)
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261 FORMAT(1H1)
262 FORMAT(1H )
    END
```

```
$IBFTC LQ1PF
C SUBPROGRAM FOR PARTITION FUNCTION OF H ATOMS
C
C THIS SUBPROGRAM FINDS THE CONTRIBUTION OF EACH EXCITED STATE TO THE
C PARTITION FUNCTION USING 2 DIFFERENT CUTOFFS AND ADOPTS THE SMALLER
C VALUE. THE CONTRIBUTIONS OF THE EXCITED STATES ARE THEN ADDED TO THE
C GROUND STATE CONTRIBUTION TO GIVE THE PARTITION FUNCTION.
      FUNCTION Q1PF(RO,DELI)
      COMMON/BLOCK2/PHI,PHIC,SUM1/BLOCK5/ARB1,ARB2
      DIMENSION PHI(17),PHIC(17),STARI(18),ROOTA(18)
      DATA STARI/10967880.,2741970.,1218650.,685490.,438720.,304670.,
     1223840.,171380.,135410.,109680.,90650.,76170.,64900.,55960.,
     248750.,42850.,37960.,33860./
      DATA ROOTA/7.2744E-6,1.4549E-5,2.1823E-5,2.9098E-5,3.6372E-5,
     14.3646E-5,5.0921E-5,5.8195E-5,6.5470E-5,7.2744E-5,8.0018E-5,
     28.7293E-5,9.4567E-5,1.0184E-4,1.0912E-4,1.1639E-4,1.2366E-4,
     31.3094E-4/
      PHIC(1)=PHI(1)
      SUM1=0.
      ROOTR= SQRT(RO*ARB1)
      DO 1 N=2,17
    2 STAR1=(STARI(N)+STARI(N+1))/2.
      IF(STAR1-DELI*ARB2)5,4,4
    4 PHIC(N)=PHI(N)
      GO TO 9
    5 IF(STARI(N)-DELI*ARB2)7,6,6
    6 PHIC(N)=PHI(N)*((STARI(N)-DELI*ARB2)/(STARI(N)-STARI(N+1))+.5)
      GO TO 9
    7 STAR2=(STARI(N-1)+STARI(N))/2.
      IF(DELI*ARB2-STAR2)8,3,3
    8 PHIC(N)=PHI(N)*((STARI(N)-DELI*ARB2)/(STARI(N-1)-STARI(N))+.5)
      GO TO 9
    3 PHIC(N)=0.
    9 ROOT1= (-ROOTA(N)-ROOTA(N+1))/2.
      IF(ROOT1+ROOTR) 11,10,10
   10 PHICN= PHI(N)
      GO TO 16
   11 IF(-ROOTA(N)+ROOTR) 13,12,12
   12 PHICN= PHI(N)*((-ROOTA(N)+ROOTR)/(-ROOTA(N)+ROOTA(N+1))+.5)
      GO TO 16
   13 ROOT2= (-ROOTA(N-1)-ROOTA(N))/2.
      IF(-ROOTR-ROOT2)14,15,15
   14 PHICN= PHI(N)*((-ROOTA(N)+ROOTR)/(-ROOTA(N-1)+ROOTA(N))+.5)
      GO TO 16
   15 PHICN= 0.
   16 PHIC(N)= AMIN1(PHIC(N),PHICN)
      SUM1= SUM1+PHIC(N)
    1 CONTINUE
      Q1PF=PHIC(1)+SUM1
      RETURN
      END
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$IBFTC LQ4PF
C SUBPROGRAM FOR PARTITION FUNCTION OF H2 MOLECULES
C
C THIS SUBPROGRAM FINDS THE CONTRIBUTION OF EACH EXCITED STATE TO THE
C PARTITION FUNCTION USING 2 DIFFERENT CUTOFFS AND ADOPTS THE SMALLER
C VALUE. THE CONTRIBUTIONS OF THE EXCITED STATES ARE THEN ADDED TO THE
C GROUND STATE CONTRIBUTION TO GIVE THE PARTITION FUNCTION.
      FUNCTION Q4PF(RO,DELI)
      COMMON/BLOCK3/SUM,GAM,GAMC,SUM4/BLOCK4/IMAX/BLOCK5/ARB1,ARB2
      DIMENSION GAM(6,23),GAMC(6,23),IMAX(23),STARI(7,23),ROOTA(7,23)
      DATA((STARI(I,J),I=1,5),J=1,3)/12441300.,2524920.,1145640.,593180.
     1,458380.,12441300.,3420970.,1393480.,752770.,458380.,12441300.,
     22531970.,1154100.,657930.,458380./
      DATA((STARI(I,J),I=1,4),J=4,6)/2892650.,1260140.,711820.,458380.,
     12892650.,1240260.,685140.,458380.,2892650.,1204780.,677040.,
     2458380./
      DATA((STARI(I,J),I=1,3),J=7,10)/1288480.,733350.,458380.,1288480.,
     1652200.,458380.,1288480.,724700.,458380.,1288480.,701600.,458380./
      DATA(STARI(I,11),I=1,5)/12441300.,2942520.,1262970.,706510.,
     1458380./
      DATA(STARI(I,12),I=1,4)/2892650.,1781960.,889930.,458380./
      DATA(STARI(I,13),I=1,5)/12441300.,2961190.,1280330.,730570.,
     1458380./
      DATA((STARI(I,J),I=1,4),J=14,16)/2892650.,1270300.,703460.,458380.
     1,2892650.,1248340.,698310.,458380.,2892650.,1211650.,692720.,
     2458380./
      DATA((STARI(I,J),I=1,3),J=17,20)/1288480.,696660.,458380.,1288480.
     1,682150.,458380.,1288480.,724760.,458380.,1288480.,701660.,
     2458380./
      DATA((STARI(I,J),I=1,7),J=21,22)/708730.,458380.,317130.,232380.,
     1177660.,140210.,113520.,140210.,113520.,93760.,78800.,67200.,
     257980.,50540./
      DATA(STARI(I,23),I=1,5)/57980.,50540.,44450.,39410.,35190./
      DATA((ROOTA(I,J),I=1,5),J=1,3)/.6803E-5,1.454E-5,2.193E-5,
     13.020E-5,3.575E-5,.6803E-5,1.312E-5,1.919E-5,2.656E-5,3.575E-5,
     2.6803E-5,1.452E-5,2.182E-5,2.882E-5,3.575E-5/
      DATA((ROOTA(I,J),I=1,4),J=4,6)/1.415E-5,2.135E-5,2.861E-5,
     13.575E-5,1.415E-5,2.150E-5,2.899E-5,3.575E-5,1.415E-5,2.194E-5,
     22.915E-5,3.575E-5/
      DATA((ROOTA(I,J),I=1,3),J=7,10)/2.120E-5,2.862E-5,3.575E-5,
     12.120E-5,2.934E-5,3.575E-5,2.120E-5,2.842E-5,3.575E-5,2.120E-5,
     22.863E-5,3.575E-5/
      DATA(ROOTA(I,11),I=1,5)/.6803E-5,1.454E-5,2.193E-5,3.020E-5,
     13.575E-5/
      DATA(ROOTA(I,12),I=1,4)/1.415E-5,1.919E-5,2.656E-5,3.575E-5/
      DATA(ROOTA(I,13),I=1,5)/.6803E-5,1.452E-5,2.182E-5,2.882E-5,
     13.575E-5/
      DATA((ROOTA(I,J),I=1,4),J=14,16)/1.415E-5,2.135E-5,2.861E-5,
     13.575E-5,1.415E-5,2.150E-5,2.899E-5,3.575E-5,1.415E-5,2.194E-5,
     22.915E-5,3.575E-5/
      DATA((ROOTA(I,J),I=1,3),J=17,20)/2.120E-5,2.862E-5,3.575E-5,
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     12.120E-5,2.934E-5,3.575E-5,2.120E-5,2.842E-5,3.575E-5,2.120E-5,
     22.863E-5,3.575E-5/
      DATA((ROOTA(I,J),I=1,7),J=21,22)/2.861E-5,3.575E-5,4.302E-5,
     15.030E-5,5.758E-5,6.485E-5,7.212E-5,6.485E-5,7.212E-5,7.940E-5,
     28.668E-5,9.395E-5,10.12E-5,10.85E-5/
      DATA(ROOTA(I,23),I=1,5)/10.12E-5,10.85E-5,11.58E-5,12.30E-5,
     113.03E-5/
      ROOTR= SQRT(RO*ARB1)
      SUM4=0.
      DO 1 M=1,23
      IMA=IMAX(M)
      DO 1 I=2,IMA
    2 STAR1=(STARI(I,M)+STARI(I+1,M))/2.
      IF(STAR1-DELI*ARB2)5,4,4
    4 GAMC(I,M)=GAM(I,M)
      GO TO 9
    5 IF(STARI(I,M)-DELI*ARB2)7,6,6
    6 GAMC(I,M)=GAM(I,M)*((STARI(I,M)-DELI*ARB2)/(STARI(I,M)-STARI(I+1,
     1M))+.5)
      GO TO 9
    7 STAR2=(STARI(I-1,M)+STARI(I,M))/2.
      IF(DELI*ARB2-STAR2)8,3,3
    8 GAMC(I,M)=GAM(I,M)*((STARI(I,M)-DELI*ARB2)/(STARI(I-1,M)-STARI(I,M
     1))+.5)
      GO TO 9
    3 GAMC(I,M)=0.
    9 ROOT1=(-ROOTA(I,M)-ROOTA(I+1,M))/2.
      IF(ROOT1+ROOTR) 11,10,10
   10 GAMCIM= GAM(I,M)
      GO TO 16
   11 IF(-ROOTA(I,M)+ROOTR) 13,12,12
   12 GAMCIM= GAM(I,M)*((-ROOTA(I,M)+ROOTR)/(-ROOTA(I,M)+ROOTA(I+1,M))
     1+.5)
      GO TO 16
   13 ROOT2= (-ROOTA(I-1,M)-ROOTA(I,M))/2.
      IF(-ROOTR-ROOT2) 14,15,15
   14 GAMCIM= GAM(I,M)*((-ROOTA(I,M)+ROOTR)/(-ROOTA(I-1,M)+ROOTA(I,M))
     1+.5)
      GO TO 16
   15 GAMCIM= 0.
   16 GAMC(I,M)= AMIN1(GAMC(I,M),GAMCIM)
      SUM4= SUM4+GAMC(I,M)
    1 CONTINUE
      Q4PF=SUM+SUM4
      RETURN
      END
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$IBFTC LBLO
C SUBPROGRAM GIVING CONSTANTS FOR H, H+, E-, H2, H-, H2+, AND H3+
C
      BLOCK DATA
      COMMON/BLOCK4/IMAX/BLOCK6/Z
     1/BLOCK7/ALPHA,EH,EF,ED,EH2,WEIGHT,RE,BETA,JP1M,KP1M,GH2,GH2P,FH2
      DIMENSION IMAX(23),Z(7),ALPHA(7),EH(17),EF(6,23),ED(6,23),EH2(6,
     123),WEIGHT(6,23),RE(6,23),BETA(6,23),JP1M(15),KP1M(20),GH2(15),
     2GH2P(20),FH2(15,39)
      DATA IMAX/4,4,4,3,3,3,2,2,2,2,4,3,4,3,3,3,2,2,2,2,6,6,4/
      DATA Z/0.,1.,1.,0.,1.,1.,1./
      DATA ALPHA/3.1673E-3,3.1700E-3,2.4940E+2,1.1198E-3,3.1649E-3,
     11.1203E-3,6.0974E-4/
      DATA EH/0.,118354.,140271.,147942.,151493.,153421.,154584.,155339.
     1,155856.,156227.,156500.,156709.,156871.,157000.,157103.,157188.,
     2157259./
      DATA EF/0.,3249.,3234.,2738.,3*0.,1918.,2382.,2935.,3*0.,3475.,
     13236.,3164.,3*0.,3342.,3269.,4*0.,3286.,3064.,4*0.,3120.,3140.,4*0
     2.,2987.,5*0.,3359.,5*0.,2979.,5*0.,3340.,5*0.,3672.,3264.,2823.,
     33*0.,3144.,3085.,4*0.,3352.,3224.,3394.,3*0.,3086.,3087.,4*0.,
     43271.,3148.,4*0.,3100.,3109.,4*0.,2953.,5*0.,3325.,5*0.,2979.,5*0.
     5,3340.,5*0.,3045.,3067.,3085.,3097.,3108.,0.,3116.,3123.,3127.,
     63130.,3133.,0.,3136.,3138.,3140.,2*0./
      DATA ED/0.,29339.,31396.,24349.,3*0.,41506.,12655.,26748.,3*0.,
     129715.,31520.,32012.,3*0.,14779.,26344.,4*0.,14464.,25847.,4*0.,
     232183.,32273.,4*0.,26497.,5*0.,25446.,5*0.,26369.,5*0.,32734.,5*0.
     3,35561.,33097.,26022.,3*0.,18642.,10362.,4*0.,35661.,33324.,
     426683.,3*0.,16026.,26123.,4*0.,15826.,26083.,4*0.,32272.,32480.,
     54*0.,25951.,5*0.,32446.,5*0.,26369.,5*0.,32735.,5*0.,29363.,
     630334.,30908.,31236.,31478.,0.,31661.,31784.,31882.,31961.,32025.
     7,.0,32072.,32112.,32147.,2*0./
      DATA EH2/0.,140975.,160835.,169035.,3*0.,128807.,157658.,166636.,
     13*0.,140751.,160711.,167890.,3*0.,159016.,167041.,4*0.,159331.,
     2167537.,4*0.,160048.,167629.,4*0.,166888.,5*0.,167843.,5*0.,
     3167016.,5*0.,167168.,5*0.,134752.,159133.,167363.,3*0.,151672.,
     4164401.,4*0.,134652.,158907.,166701.,3*0.,159045.,167261.,4*0.,
     5159245.,167301.,4*0.,159959.,167422.,4*0.,167433.,5*0.,167456.,
     65*0.,167015.,5*0.,167167.,5*0.,170820.,172843.,174053.,174835.,
     7175369.,0.,175749.,176030.,176243.,176408.,176540.,0.,176645.,
     8176732.,176803.,2*0./
      DATA WEIGHT/0.,3*1.,3*0.,3*1.,3*0.,3*2.,3*0.,2*1.,4*0.,2*2.,4*0.,
     12*2.,4*0.,1.,5*0.,2.,5*0.,2.,5*0.,2.,5*0.,3*3.,3*0.,2*3.,4*0.,
     23*6.,3*0.,2*3.,4*0.,2*6.,4*0.,2*6.,4*0.,3.,5*0.,6.,5*0.,6.,5*0.,
     36.,5*0.,100.,144.,196.,256.,324.,0.,400.,484.,576.,676.,784.,0.,
     4900.,1024.,1156.,2*0./
      DATA RE/0.,1.0334E-10,1.1181E-10,1.1290E-10,3*0.,1.2907E-10,
     11.1270E-10,1.111E-10,3*0.,1.0316E-10,1.0440E-10,1.0555E-10,3*0.,
     21.0740E-10,1.4205E-10,4*0.,1.1639E-10,1.3972E-10,4*0.,.9916E-10,
     3.8959E-10,4*0.,1.0809E-10,5*0.,1.0583E-10,5*0.,1.0821E-10,5*0.,
     41.0253E-10,5*0.,.9955E-10,1.0613E-10,1.1132E-10,3*0.,1.0869E-10,
     51.0654E-10,4*0.,1.0499E-10,1.0667E-10,1.0603E-10,3*0.,1.4461E-10,
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6.9298E-10,4*0.,1.1466E-10,1.1675E-10,4*0.,.9937E-10,.8348E-10,
74*0.,1.0866E-10,5*0.,1.0276E-10,5*0.,1.0821E-10,5*0.,1.0253E-10,
85*0.,1.0732E-10,1.0703E-10,1.0676E-10,1.0657E-10,1.0641E-10,0.,
91.0628E-10,1.0617E-10,1.0610E-10,1.0605E-10,1.0600E-10,0.,
A1.0595E-10,1.0592E-10,1.0589E-10,2*0./
 DATA BETA/0.,1.4529E+10,1.3907E+10,1.3448E+10,3*0.,.6948E+10,
11.7070E+10,1.3750E+10,3*0.,1.5493E+10,1.3895E+10,1.3451E+10,3*0.,
22.2770E+10,1.5551E+10,4*0.,2.2658E+10,1.4662E+10,4*0.,1.3204E+10,
31.3281E+10,4*0.,1.4068E+10,5*0.,1.6348E+10,5*0.,1.4068E+10,5*0.,
41.4068E+10,5*0.,1.4844E+10,1.3641E+10,1.3385E+10,3*0.,1.8309E+10,
52.6694E+10,4*0.,1.3497E+10,1.3407E+10,1.6084E+10,3*0.,1.9680E+10,
61.4693E+10,4*0.,2.1220E+10,1.5022E+10,4*0.,1.3103E+10,1.3086E+10,
74*0.,1.4068E+10,5*0.,1.4068E+10,5*0.,1.4068E+10,5*0.,1.4068E+10,
85*0.,1.3556E+10,1.3406E+10,1.3352E+10,1.3330E+10,1.3319E+10,0.,
91.3314E+10,1.3311E+10,1.3309E+10,1.3308E+10,1.3307E+10,0.,
A3*1.3307E+10,2*0./
 DATA JP1M/39,36,34,32,30,28,26,24,22,19,17,15,12,9,5/,KP1M/42,40,
138,37,35,33,31,30,28,26,24,22,20,18,16,14,11,8,5,2/
 DATA GH2/0.,416114.,808574.,1178092.,1524910.,1849093.,2150499.,
22428777.,2683139.,2912441.,3115129.,3288751.,3430366.,3535284.,
23597480./,GH2P/0.,219134.,425545.,619656.,801821.,972336.,
31131427.,1279260.,1415937.,1541490.,1655879.,1758991.,1850623.,
41930484.,1998171.,2053168.,2094829.,2122424.,2135548.,2137849./
 DATA ( FH2  (I, 1),I=1,15)/
X       0.,       0.,      -0.,      -0.,      -0.,       0.,
X       0.,      -0.,       0.,      -0.,      -0.,       0.,
X      -0.,      -0.,       0./
 DATA ( FH2  (I, 2),I=1,15)/
X    11852.,    11257.,    10679.,    10111.,     9565.,     8988.,
X     8413.,     7821.,     7211.,     6557.,     5849.,     5068.,
X     4152.,     3079.,     1727./
 DATA ( FH2  (I, 3),I=1,15)/
X    35453.,    33672.,    31932.,    30233.,    28582.,    26865.,
X    25136.,    23363.,    21527.,    19579.,    17463.,    15123.,
X    12365.,     9114.,     4994./
 DATA ( FH2  (I, 4),I=1,15)/
X    70587.,    67029.,    63564.,    60171.,    56881.,    53456.,
X    50009.,    46467.,    42801.,    38910.,    34663.,    29976.,
X    24489.,    17879.,     9439./
 DATA ( FH2  (I, 5),I=1,15)/
X   116932.,   111037.,   105286.,    99643.,    94162.,    88500.,
X    82760.,    76875.,    70757.,    64279.,    57196.,    49365.,
X    40218.,    29090.,    14500./
 DATA ( FH2  (I, 6),I=1,14)/
X   174094.,   165299.,   156715.,   148294.,   140077.,   131651.,
X   123062.,   114259.,   105089.,    95367.,    84730.,    72917.,
X    59127.,    42240./
 DATA ( FH2  (I, 7),I=1,14)/
X   241600.,   229358.,   217404.,   205686.,   194196.,   182501.,
X   170530.,   158230.,   145398.,   131803.,   116864.,   100218.,
X    80722.,    56691./
 DATA ( FH2  (I, 8),I=1,14)/
X   318852.,   302680.,   286854.,   271338.,   256050.,   240547.,
X   224697.,   208344.,   191254.,   173066.,   153109.,   130746.,
X   104418.,    71609./
 DATA ( FH2  (I, 9),I=1,14)/
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X  405346.,  384685.,  364505.,  344702.,  325119.,  305303.,
X  285058.,  264112.,  242156.,  218740.,  192981.,  163947.,
X  129518.,   85558./
 DATA ( FH2  (I,10),I=1,13)/
X  500392.,  474767.,  449781.,  425219.,  400851.,  376206.,
X  351079.,  325015.,  297609.,  268282.,  235916.,  199246.,
X  155153./
 DATA ( FH2  (I,11),I=1,13)/
X  603335.,  572282.,  542057.,  512290.,  482679.,  452715.,
X  422177.,  390486.,  357056.,  321116.,  281300.,  235841.,
X  180225./
 DATA ( FH2  (I,12),I=1,13)/
X  713500.,  676570.,  640698.,  605301.,  569997.,  534273.,
X  497810.,  459917.,  419866.,  376580.,  328393.,  272721.,
X  203042./
 DATA ( FH2  (I,13),I=1,12)/
X  830194.,  786987.,  745062.,  703666.,  662221.,  620288.,
X  577390.,  532733.,  485385.,  433965.,  376318.,  308806./
 DATA ( FH2  (I,14),I=1,12)/
X  952734.,  902894.,  854558.,  806738.,  758744.,  710158.,
X  660331.,  608326.,  553002.,  492575.,  424316.,  342614./
 DATA ( FH2  (I,15),I=1,12)/
X 1080441., 1023684.,  968516.,  913920.,  858987.,  803306.,
X  746059.,  686133.,  622111.,  551738.,  471342.,  371564./
 DATA ( FH2  (I,16),I=1,11)/
X 1212683., 1148721., 1086399., 1024604.,  962369.,  899130.,
X  833977.,  765532.,  691994.,  610507.,  515770./
 DATA ( FH2  (I,17),I=1,11)/
X 1348894., 1277402., 1207582., 1138229., 1068309.,  997097..
X  923479.,  845805.,  761758.,  667760.,  555461./
 DATA ( FH2  (I,18),I=1,10)/
X 1488465., 1409142., 1331524., 1254241., 1176241., 1096586.,
X 1013929.,  926305.,  830773.,  722407./
 DATA ( FH2  (I,19),I=1,10)/
X 1630829., 1543379., 1457681., 1372094., 1285621., 1197038.,
X 1104753., 1006324.,  897973.,  772062./
 DATA ( FH2  (I,20),I=1, 9)/
X 1775451., 1679592., 1585510., 1491280., 1395881., 1297904.,
X 1195296., 1084950.,  961921./
 DATA ( FH2  (I,21),I=1, 9)/
X 1921791., 1817272., 1714504., 1611313., 1506573., 1398545.,
X 1284780., 1161330., 1020958./
 DATA ( FH2  (I,22),I=1, 9)/
X 2069372., 1955961., 1844169., 1731686., 1617105., 1498380.,
X 1372526., 1234226., 1070223./
 DATA ( FH2  (I,23),I=1, 8)/
X 2217699., 2095209., 1974039., 1851871., 1726957., 1596827.,
X 1457534., 1301644./
 DATA ( FH2  (I,24),I=1, 8)/
X 2366299., 2234566., 2103658., 1971389., 1835555., 1693041.,
X 1538665., 1359827./
 DATA ( FH2  (I,25),I=1, 7)/
X 2514773., 2373579., 2232613., 2089735., 1942227., 1786214.,
X 1614187./
 DATA ( FH2  (I,26),I=1, 7)/
X 2662745., 2511826., 2360462., 2206391., 2046374., 1875100.,
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X 1680320./
 DATA ( FH2  (I,27),I=1, 6)/
X 2809896., 2648894., 2486726., 2320839., 2147107., 1958130./
 DATA ( FH2  (I,28),I=1, 6)/
X 2955879., 2784347., 2610949., 2432370., 2243405., 2031554./
 DATA ( FH2  (I,29),I=1, 5)/
X 3100329., 2917813., 2732578., 2540291., 2333484./
 DATA ( FH2  (I,30),I=1, 5)/
X 3242913., 3048916., 2851009., 2643523., 2414117./
 DATA ( FH2  (I,31),I=1, 4)/
X 3383239., 3177186., 2965595., 2740537./
 DATA ( FH2  (I,32),I=1, 4)/
X 3520920., 3302143., 3075429., 2828060./
 DATA ( FH2  (I,33),I=1, 3)/
X 3655593., 3423200., 3179162./
 DATA ( FH2  (I,34),I=1, 3)/
X 3786839., 3539599., 3273966./
 DATA ( FH2  (I,35),I=1, 2)/
X 3914204., 3650081./
 DATA ( FH2  (I,36),I=1, 2)/
X 4037023., 3752564./
 DATA ( FH2  (I,37),I=1, 1)/
X 4154504./
 DATA ( FH2  (I,38),I=1, 1)/
X 4265188./
 DATA ( FH2  (I,39),I=1, 1)/
X 4364780./
 END
```

```
$IBFTC LBLP
C SUBPROGRAM GIVING CONSTANTS FOR H2+, H3+, AND DIATOMIC PARTITION
C FUNCTION APPROXIMATION USED FOR H2*
C
      BLOCK DATA
      COMMON/BLOCK8/FH2P,Q7PT,TT,THETAT,WOT,W1T,W2T
      DIMENSION FH2P(20,42),Q7PT(67),TT(67),THETAT(29),WOT(29),W1T(29),
     1W2T(29)
      DATA ( FH2P (I, 1),I=1,20)/
     X     -0.,         -0.,         -0.,          0.,          0.,         -0.,
     X      0.,         -0.,         -0.,          0.,          0.,         -0.,
     X      0.,         -0.,          0.,          0.,          0.,          0.,
     X     -0.,          0./
      DATA ( FH2P (I, 2),I=1,20)/
     X   5826.,       5519.,       5221.,       4936.,       4656.,       4384.,
     X   4110.,       3845.,       3579.,       3313.,       3044.,       2770.,
     X   2484.,       2193.,       1884.,       1554.,       1192.,        790.,
     X    342.,         63./
      DATA ( FH2P (I, 3),I=1,19)/
     X  17418.,      16511.,      15626.,      14773.,      13951.,      13101.,
     X  12309.,      11501.,      10702.,       9895.,       9106.,       8268.,
     X   7432.,       6548.,       5624.,       4627.,       3542.,       2328.,
     X    950./
      DATA ( FH2P (I, 4),I=1,19)/
     X  34714.,      32891.,      31125.,      29420.,      27761.,      26098.,
     X  24499.,      22896.,      21305.,      19702.,      18110.,      16462.,
     X  14769.,      13006.,      11153.,       9159.,       6981.,       4537.,
     X   1771./
      DATA ( FH2P (I, 5),I=1,19)/
     X  57562.,      54529.,      51597.,      48763.,      45996.,      43255.,
     X  40588.,      37931.,      35288.,      32627.,      29971.,      27233.,
     X  24414.,      21477.,      18367.,      15053.,      11405.,       7290.,
     X   2567./
      DATA ( FH2P (I, 6),I=1,18)/
     X  85804.,      81259.,      76880.,      72653.,      68504.,      64428.,
     X  60438.,      56481.,      52536.,      48568.,      44569.,      40470.,
     X  36248.,      31846.,      27178.,      22158.,      16674.,      10415./
      DATA ( FH2P (I, 7),I=1,18)/
     X 119199.,     112880.,     106783.,     100893.,      95115.,      89449.,
     X  83891.,      78374.,      72874.,      67340.,      61754.,      56032.,
     X  50126.,      43966.,      37415.,      30368.,      22612.,      13667./
      DATA ( FH2P (I, 8),I=1,18)/
     X 157500.,     149161.,     141087.,     133252.,     125623.,     118125.,
     X 110752.,     103434.,      96132.,      88791.,      81362.,      73750.,
     X  65887.,      57670.,      48936.,      39471.,      28995.,      16648./
      DATA ( FH2P (I, 9),I=1,17)/
     X 200508.,     189847.,     179545.,     169572.,     159802.,     150242.,
     X 140817.,     131465.,     122124.,     112715.,     103195.,      93443.,
     X  83341.,      72772.,      61500.,      49244.,      35545./
      DATA ( FH2P (I,10),I=1,17)/
     X 247871.,     234658.,     221891.,     209501.,     197419.,     185550.,
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X   173848.,   162231.,   150619.,   138934.,   127075.,   114906.,
X   102289.,    89046.,    74899.,    59454.,    41872./
 DATA ( FH2P (I,11),I=1,17)/
X   299287.,   283321.,   267857.,   252860.,   238213.,   223821.,
X   209629.,   195526.,   181418.,   167178.,   152762.,   137909.,
X   122509.,   106286.,    88881.,    69717.,    47436./
 DATA ( FH2P (I,12),I=1,16)/
X   354507.,   335523.,   317158.,   299338.,   281915.,   264794.,
X   247890.,   231081.,   214267.,   197292.,   180031.,   162258.,
X   143766.,   124214.,   103156.,    79723./
 DATA ( FH2P (I,13),I=1,16)/
X   413131.,   390969.,   369504.,   348652.,   328260.,   308204.,
X   288397.,   268687.,   248932.,   228981.,   208650.,   187679.,
X   165801.,   142591.,   117391.,    88908./
 DATA ( FH2P (I,14),I=1,16)/
X   474906.,   449325.,   424587.,   400526.,   376973.,   353795.,
X   330899.,   308056.,   285182.,   261999.,   238367.,   213926.,
X   188320.,   161065.,   131180.,    96138./
 DATA ( FH2P (I,15),I=1,15)/
X   539480.,   510340.,   482122.,   454676.,   427770.,   401295.,
X   375092.,   348967.,   322728.,   296142.,   268931.,   240735.,
X   211086.,   179298.,   143982./
 DATA ( FH2P (I,16),I=1,15)/
X   606555.,   573682.,   541824.,   510823.,   480405.,   450453.,
X   420801.,   391179.,   361384.,   331113.,   300078.,   267822.,
X   233725.,   196869.,   154868./
 DATA ( FH2P (I,17),I=1,14)/
X   675813.,   639063.,   603420.,   568673.,   534604.,   501009.,
X   467684.,   434374.,   400829.,   366666.,   331539.,   294877.,
X   255913.,   213220./
 DATA ( FH2P (I,18),I=1,14)/
X   746961.,   706187.,   666609.,   628013.,   590104.,   552705.,
X   515559.,   478369.,   440836.,   402539.,   363021.,   321573.,
X   277166.,   227433./
 DATA ( FH2P (I,19),I=1,13)/
X   819714.,   774786.,   731121.,   688521.,   646665.,   605298.,
X   564153.,   522908.,   481149.,   438458.,   394216.,   347533.,
X   296924./
 DATA ( FH2P (I,20),I=1,13)/
X   893796.,   844572.,   796731.,   750004.,   704026.,   658540.,
X   613226.,   567696.,   521531.,   474135.,   424794.,   372301.,
X   314226./
 DATA ( FH2P (I,21),I=1,12)/
X   968947.,   915328.,   863177.,   812177.,   761957.,   712195.,
X   662532.,   612526.,   561662.,   509262.,   454356.,   395284./
 DATA ( FH2P (I,22),I=1,12)/
X  1044880.,   986793.,   930222.,   874836.,   820241.,   766038.,
X   711857.,   657127.,   601295.,   543481.,   482431.,   415404./
 DATA ( FH2P (I,23),I=1,11)/
X  1121411.,  1058739.,   997639.,   937744.,   878605.,   819813.,
X   760888.,   701235.,   640093.,   576436.,   508364./
 DATA ( FH2P (I,24),I=1,11)/
X  1198293.,  1130945.,  1065209.,  1000683.,   936873.,   873310.,
X   809445.,   744572.,   677761.,   607587.,   531009./
 DATA ( FH2P (I,25),I=1,10)/
X  1275312.,  1203199.,  1132724.,  1063444.,   994828.,   926300.,
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X  857250.,   786830.,   713829.,   636234./
 DATA ( FH2P (I,26),I=1,10)/
X 1352270., 1275300., 1199980., 1125842., 1052205.,  978528.,
X  904028.,  827675.,  747830.,  661026./
 DATA ( FH2P (I,27),I=1, 9)/
X 1428972., 1347059., 1266786., 1187602., 1108834., 1029763.,
X  949478.,  866633.,  778916./
 DATA ( FH2P (I,28),I=1, 9)/
X 1505235., 1418292., 1332947., 1248595., 1164471., 1079732.,
X  993247.,  903208.,  805429./
 DATA ( FH2P (I,29),I=1, 8)/
X 1580909., 1488816., 1398277., 1308589., 1218877., 1128133.,
X 1034872.,  936456./
 DATA ( FH2P (I,30),I=1, 8)/
X 1655766., 1558459., 1462588., 1367370., 1271798., 1174615.,
X 1073797.,  964079./
 DATA ( FH2P (I,31),I=1, 7)/
X 1729725., 1627072., 1525687., 1424714., 1322934., 1218714.,
X 1108939./
 DATA ( FH2P (I,32),I=1, 6)/
X 1802543., 1694420., 1587375., 1480369., 1371923., 1259755./
 DATA ( FH2P (I,33),I=1, 6)/
X 1874138., 1760389., 1647441., 1534041., 1418290., 1296477./
 DATA ( FH2P (I,34),I=1, 5)/
X 1944330., 1824775., 1705651., 1585373., 1461285./
 DATA ( FH2P (I,35),I=1, 5)/
X 2012959., 1887378., 1761698., 1633861., 1499343./
 DATA ( FH2P (I,36),I=1, 4)/
X 2079863., 1947977., 1815243., 1678677./
 DATA ( FH2P (I,37),I=1, 4)/
X 2144863., 2006299., 1865786., 1717821./
 DATA ( FH2P (I,38),I=1, 3)/
X 2207751., 2062003., 1912420./
 DATA ( FH2P (I,39),I=1, 2)/
X 2268294., 2114594./
 DATA ( FH2P (I,40),I=1, 2)/
X 2326179., 2163145./
 DATA ( FH2P (I,41),I=1, 1)/
X 2380966./
 DATA ( FH2P (I,42),I=1, 1)/
X 2431910./
 DATA Q7PT/4.8506,7.4266,1.0359E+1,1.3623E+1,1.7220E+1,2.1167E+1,
12.5503E+1,3.0275E+1,3.5544E+1,4.1372E+1,4.7830E+1,5.4991E+1,
26.2936E+1,7.1746E+1,8.1509E+1,9.2319E+1,1.0427E+2,1.1748E+2,
31.4809E+2,1.8511E+2,2.2965E+2,2.8294E+2,3.4637E+2,4.2149E+2,
45.1005E+2,6.1401E+2,7.3555E+2,8.7712E+2,1.1331E+3,1.4509E+3,
51.8428E+3,2.3235E+3,3.1320E+3,4.1768E+3,5.9064E+3,8.2440E+3,
61.1374E+4,1.5520E+4,2.0951E+4,2.7988E+4,3.7011E+4,4.8460E+4,
78.0735E+4,1.2969E+5,2.0129E+5,3.0243E+5,4.4063E+5,6.2364E+5,
88.5881E+5,1.1525E+6,1.5091E+6,1.9310E+6,2.9635E+6,4.2018E+6,
95.5432E+6,6.8387E+6,8.2173E+6,9.6610E+6,1.1154E+7,1.2682E+7,
A1.4233E+7,1.5797E+7,1.8147E+7,2.0485E+7,2.2790E+7,2.5052E+7,
B2.7985E+7/
 DATA TT/300.,400.,500.,600.,700.,800.,900.,1000.,1100.,1200.,
11300.,1400.,1500.,1600.,1700.,1800.,1900.,2000.,2200.,2400.,2600.
2,2800.,3000.,3200.,3400.,3600.,3800.,4000.,4300.,4600.,4900.,
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35200.,5600.,6000.,6500.,7000.,7500.,8000.,8500.,9000.,9500.,
410000.,11000.,12000.,13000.,14000.,15000.,16000.,17000.,18000.,
519000.,20000.,22000.,24000.,26000.,28000.,30000.,32000.,34000.,
636000.,38000.,40000.,43000.,46000.,49000.,52000.,56000./
 DATA THETAT/.030,.035,.040,.050,.060,.070,.080,.100,.130,.16,.20,
1.25,.30,.35,.4,.5,.6,.7,.8,1.0,1.3,1.6,2.0,2.5,3.0,3.5,4.,5.,6./,
2WOT/2.7634E-1,2.9930E-1,3.2085E-1,3.6077E-1,3.9754E-1,4.3202E-1,
34.6477E-1,5.2644E-1,6.1114E-1,6.8566E-1,7.6545E-1,8.3158E-1,
48.6490E-1,8.7356E-1,8.6530E-1,8.2038E-1,7.5978E-1,6.9697E-1,
56.3748E-1,5.3465E-1,4.1907E-1,3.3762E-1,2.6264E-1,2.0105E-1,
61.6003E-1,1.3119E-1,1.1004E-1,8.1486E-2,6.3428E-2/,W1T/6.5423E-3,
78.3437E-3,1.0320E-2,1.4798E-2,1.9991E-2,2.5941E-2,3.2704E-2,
84.8882E-2,7.9674E-2,1.1599E-1,1.6618E-1,2.2169E-1,2.6369E-1,
92.9218E-1,3.0945E-1,3.2083E-1,3.1439E-1,2.9978E-1,2.8200E-1,
A2.4567E-1,1.9914E-1,1.6373E-1,1.2958E-1,1.0054E-1,8.0733E-2,
B6.6599E-2,5.6119E-2,4.1828E-2,3.2698E-2/,W2T/4.6888E-3,6.0577E-3,
C7.5925E-3,1.1192E-2,1.5575E-2,2.0878E-2,2.7282E-2,4.4229E-2,
D8.1832E-2,1.3254E-1,2.1022E-1,3.0404E-1,3.8063E-1,4.3657E-1,
E4.7393E-1,5.0763E-1,5.0774E-1,4.9096E-1,4.6657E-1,4.1208E-1,
F3.3815E-1,2.8008E-1,2.2305E-1,1.7391E-1,1.4011E-1,1.1586E-1,
G9.7787E-2,7.3060E-2,5.7204E-2/
 END
```

```
$IBFTC LMATR    DEBUG
C SUBPROGRAM TO FIND MATRIX AND INITIAL VECTOR FOR ITERATIVE CORRECTIONS
C
C THIS SUBPROGRAM FINDS 1ST DERIVATIVES OF PRESSURE WITH RESPECT TO
C MOLES AND VOLUME AND 1ST AND 2ND DERIVATIVES OF FREE ENERGY WITH
C RESPECT TO MOLES AND VOLUME. FROM THESE IT FINDS THE 5X5 MATRIX X AND
C INITIAL VECTOR Y FOR ITERATIVE CORRECTIONS.
      SUBROUTINE MATR(V,GMO,S,ETA,C,Q,ROOT,SUMM,SM,X,Y,SN,SV)
      COMMON/BLOCK1/DH,T,PO,PROD,ETAD,SD/BLOCK6/Z
      DOUBLE PRECISION V,GMO(7),SN(2),SV,FN(7),FV,FVV,FNV(7),FNN(7,7),
     1X(5,5),Y(5),SM,ROOT,SUMM,PRODD,S,ETA,C,PRODDD,RES,W,SN1SV,SN2SV
      DIMENSION PROD(7),Q(7),Z(7)
      SN(1)= 8.3143*T/(PO*V)
      SN(2)= SN(1)-3.4733D3*DH*ROOT/(PO*V)
      SV= -8.3143*T*SUMM/(PO*V**2)+.27465*DH*T*ROOT**3/(PO*V)
      PRODD= 9.9100D-2*DSQRT((1.2646D4/T)**3*SM/V)
      DO 3 L=1,7
    3 FN(L)= -DLOG(V*Q(L)/(PROD(L)*GMO(L)))+1.-Z(L)*PRODD*DH
      DEBUG SN(1),SN(2),SV,(FN(I),I=1,7)
      FV= -SUMM/V+.033033*ROOT**3*DH
      FVV=SUMM/V**2-.049550*ROOT**3*DH/V
      PRODDD= .049550*(1.2646D4/(T*V))**1.5D0*DSQRT(SM)
      DO 4 M=1,7
    4 FNV(M)= -1./V+Z(M)*PRODDD*DH
      RES= .049550*DSQRT((1.2646D4/T)**3/(V*SM))
      DEBUG FV,FVV,(FNV(I),I=1,7)
      DO 5 I=1,7
      DO 5 N=1,7
      IF (I-N) 7,6,7
    6 FNN(I,N)= 1./GMO(I)-Z(I)*RES*DH
      GO TO 5
    7 FNN(I,N)= -Z(I)*Z(N)*RES*DH
    5 CONTINUE
      W= (SD-S+C*SN(2)-.5D0*SN(1)*(ETAD-ETA))/SV
      SN1SV= SN(1)/SV
      SN2SV= SN(2)/SV
      DEBUG W,SN1SV,SN2SV,((FNN(I,N),N=I,7),I=1,7)
      X(1,1)=(FNN(1,1)+.25D0*FNN(4,4)+SN1SV*(.25D0*SN1SV*FVV-FNV(1)+.5D0
     1*FNV(4))-FNN(1,4))*GMO(1)
      X(1,2)=(.25D0*FNN(4,4)+SN1SV*((-.25D0*SN1SV+SN2SV)*FVV-.5D0*FNV(2)
     1-.5D0*FNV(3)+.5D0*FNV(1))-2.*SN2SV*(FNV(1)-.5D0*FNV(4))+FNN(1,2)+
     2FNN(1,3)-.5D0*FNN(1,4)-.5D0*FNN(2,4)-.5D0*FNN(3,4))*GMO(2)
      X(1,3)=(.25D0*FNN(4,4)+SN1SV*(-.25D0*SN1SV*FVV+.5D0*FNV(3)-.5D0*
     1FNV(5)+.5D0*FNV(1))-FNN(1,3)-.5D0*FNN(1,4)+FNN(1,5)+.5D0*FNN(3,4)-
     2.5D0*FNN(4,5))*GMO(5)
      X(1,4)=(.5D0*FNN(4,4)+SN1SV*((SN2SV-.5D0*SN1SV)*FVV-.5D0*FNV(3)-
     1.5D0*FNV(6)+FNV(1))-2.*SN2SV*(FNV(1)-.5D0*FNV(4))+FNN(1,3)-FNN(1,4
     2)+FNN(1,6)-.5D0*FNN(3,4)-.5D0*FNN(4,6))*GMO(6)
      X(1,5)=(.75D0*FNN(4,4)+SN1SV*((-.75D0*SN1SV+SN2SV)*FVV-.5D0*FNV(3)
     1+1.5D0*FNV(1)-.5D0*FNV(7))+SN2SV*(-2.*FNV(1)+FNV(4))+FNN(1,3)-1.5D
     20*FNN(1,4)+FNN(1,7)-.5D0*FNN(3,4)-.5D0*FNN(4,7))*GMO(7)
```

```
 Y(1)=-(FN(1)-.5D0*FN(4)-.5D0*SN1SV*FV+(ETAD-ETA)*(-.25D0*FNN(4,4)-
1.25D0*SN1SV*FNV(4)+.5D0*FNN(1,4))-W*.5D0*SN1SV*FVV+W*(FNV(1)-.5D0*
2FNV(4))+C*(.5D0*SN1SV*FNV(3)-FNN(1,3)+.5D0*FNN(3,4)))
 X(2,1)=(.25D0*FNN(4,4)+SN1SV*((-.25D0*SN1SV+SN2SV)*FVV-.5D0*FNV(2)
1-.5D0*FNV(3)+.5D0*FNV(1))+SN2SV*(-2.*FNV(1)+FNV(4))+FNN(1,2)+
2FNN(1,3)-.5D0*FNN(1,4)-.5D0*FNN(2,4)-.5D0*FNN(3,4))*GMO(1)
 X(2,2)=(FNN(2,2)+FNN(3,3)+.25D0*FNN(4,4)+(.5D0*SN1SV-2.*SN2SV)**2*
1FVV+(SN1SV-4.*SN2SV)*(FNV(2)+FNV(3)-.5D0*FNV(4))+2.*FNN(2,3)-
2FNN(2,4)-FNN(3,4))*GMO(2)
 X(2,3)=(-FNN(3,3)+.25D0*FNN(4,4)+SN1SV*((.25D0*SN1SV-SN2SV)*FVV-
1.5D0*FNV(4)+.5D0*FNV(2)+.5D0*FNV(5))+SN2SV*(2.*FNV(3)-2.*FNV(5)+
2FNV(4))-FNN(2,3)-.5D0*FNN(2,4)+FNN(2,5)+FNN(3,5)-.5D0*FNN(4,5))*
3GMO(5)
 X(2,4)=(FNN(3,3)+.5D0*FNN(4,4)+(.5D0*SN1SV-2.*SN2SV)*(SN1SV-2.*
1SN2SV)*FVV+SN1SV*(1.5D0*FNV(3)-FNV(4)+FNV(2)+.5D0*FNV(6))+SN2SV*(-
24.*FNV(3)+3.*FNV(4)-2.*FNV(2)-2.*FNV(6))+FNN(2,3)-FNN(2,4)+FNN(2,6
3)-1.5D0*FNN(3,4)+FNN(3,6)-.5D0*FNN(4,6))*GMO(6)
 X(2,5)=(FNN(3,3)+.75D0*FNN(4,4)+(.5D0*SN1SV-2.*SN2SV)*(1.5D0*SN1SV
1-2.*SN2SV)*FVV+SN1SV*(2.*FNV(3)-1.5D0*FNV(4)+1.5D0*FNV(2)+.5D0*
2FNV(7))+SN2SV*(-4.*FNV(3)+4.*FNV(4)-2.*FNV(2)-2.*FNV(7))+FNN(2,3)-
31.5D0*FNN(2,4)+FNN(2,7)-2.*FNN(3,4)-.5D0*FNN(4,7)+FNN(3,7))*GMO(7)
 Y(2)=-(FN(2)+FN(3)-.5D0*FN(4)+FV*(.5D0*SN1SV-2.*SN2SV)+C*(-FNN(3,3
1)-(.5D0*SN1SV-2.*SN2SV)*FNV(3)-FNN(2,3)+.5D0*FNN(3,4))+(ETAD-ETA)*
2(-.25D0*FNN(4,4)+(.25D0*SN1SV-SN2SV)*FNV(4)+.5D0*FNN(2,4)+.5D0*
3FNN(3,4))+W*(.5D0*SN1SV-2.*SN2SV)*FVV+W*(FNV(2)+FNV(3)-.5D0*FNV(4)
4))
 X(3,1)=(.25D0*FNN(4,4)+SN1SV*(-.25D0*SN1SV*FVV+.5D0*FNV(3)-.5D0*
1FNV(5)+.5D0*FNV(1))-FNN(1,3)-.5D0*FNN(1,4)+FNN(1,5)+.5D0*FNN(3,4)-
2.5D0*FNN(4,5))*GMO(1)
 X(3,2)=(-FNN(3,3)+.25D0*FNN(4,4)+SN1SV*((.25D0*SN1SV-SN2SV)*FVV-
1.5D0*FNV(4)+.5D0*FNV(2)+.5D0*FNV(5))+SN2SV*(2.*FNV(3)-2.*FNV(5)+
2FNV(4))-FNN(2,3)-.5D0*FNN(2,4)+FNN(2,5)+FNN(3,5)-.5D0*FNN(4,5))*
3GMO(2)
 X(3,3)=(FNN(3,3)+.25D0*FNN(4,4)+FNN(5,5)+SN1SV*(.25D0*SN1SV*FVV-
1FNV(3)+FNV(5)-.5D0*FNV(4))+FNN(3,4)-2.*FNN(3,5)-FNN(4,5))*GMO(5)
 X(3,4)=(-FNN(3,3)+.5D0*FNN(4,4)+SN1SV*(.5D0*(SN1SV-2.*SN2SV)*FVV
1-.5D0*FNV(3)+.5D0*FNV(6)-FNV(4)+FNV(5))+SN2SV*(2.*FNV(3)-2.*
2FNV(5)+FNV(4))+.5D0*FNN(3,4)-FNN(4,5)-.5D0*FNN(4,6)+FNN(5,6)+
3FNN(3,5)-FNN(3,6))*GMO(6)
 X(3,5)=(-FNN(3,3)+.75D0*FNN(4,4)+SN1SV*((.75D0*SN1SV-SN2SV)*FVV-
1FNV(3)-1.5D0*FNV(4)+1.5D0*FNV(5)+.5D0*FNV(7))+SN2SV*(2.*FNV(3)-2.
2*FNV(5)+FNV(4))+FNN(3,4)+FNN(3,5)-1.5D0*FNN(4,5)-.5D0*FNN(4,7)+
3FNN(5,7)-FNN(3,7))*GMO(7)
 Y(3)=-(-FN(3)-.5D0*FN(4)+FN(5)+.5D0*SN1SV*FV+C*(FNN(3,3)-.5D0*
1SN1SV*FNV(3)+.5D0*FNN(3,4)-FNN(3,5))+(ETAD-ETA)*(-.25D0*FNN(4,4)+
2.25D0*SN1SV*FNV(4)-.5D0*FNN(3,4)+.5D0*FNN(4,5))+W*.5D0*SN1SV*FVV+
3W*(FNV(5)-FNV(3)-.5D0*FNV(4)))
 X(4,1)=(.5D0*FNN(4,4)+SN1SV*((-.5D0*SN1SV+SN2SV)*FVV-.5D0*FNV(3)-
1.5D0*FNV(6)+FNV(1))-2.*SN2SV*(FNV(1)-.5D0*FNV(4))+FNN(1,3)-FNN(1,4
2)+FNN(1,6)-.5D0*FNN(3,4)-.5D0*FNN(4,6))*GMO(1)
 X(4,2)=(FNN(3,3)+.5D0*FNN(4,4)+(.5D0*SN1SV-2.*SN2SV)*(SN1SV-2.*
1SN2SV)*FVV+SN1SV*(1.5D0*FNV(3)-FNV(4)+FNV(2)+.5D0*FNV(6))+SN2SV*
2(-4.*FNV(3)+3.*FNV(4)-2.*FNV(2)-2.*FNV(6))+FNN(2,3)-FNN(2,4)+
3FNN(2,6)-1.5D0*FNN(3,4)+FNN(3,6)-.5D0*FNN(4,6))*GMO(2)
 X(4,3)=(-FNN(3,3)+.5D0*FNN(4,4)+SN1SV*((.5D0*SN1SV-SN2SV)*FVV+
1FNV(5)+.5D0*FNV(3)-.5D0*FNV(4)+.5D0*FNV(6)-FNV(3)-.5D0*FNV(4))+
```

```
2SN2SV*(2.*FNV(3)-2.*FNV(5)+FNV(4))+.5D0*FNN(3,4)-FNN(4,5)-.5D0*
3FNN(4,6)+FNN(5,6)+FNN(3,5)-FNN(3,6))*GMO(5)
 X(4,4)=(FNN(3,3)+FNN(4,4)+FNN(6,6)+(SN1SV-2.*SN2SV)**2*FVV+2.*(
1SN1SV-2.*SN2SV)*(FNV(3)+FNV(6)-FNV(4))-2.*FNN(3,4)+2.*FNN(3,6)-2.
2*FNN(4,6))*GMO(6)
 X(4,5)=(FNN(3,3)+1.5D0*FNN(4,4)+(SN1SV-2.*SN2SV)*(1.5D0*SN1SV-2.*
1SN2SV)*FVV+SN1SV*(1.5D0*FNV(6)-3.*FNV(4)+2.5D0*FNV(3)+FNV(7))+
2SN2SV*(-4.*FNV(3)+5.*FNV(4)-2.*FNV(6)-2.*FNV(7))-2.5D0*FNN(3,4)+
3FNN(3,6)-1.5D0*FNN(4,6)-FNN(4,7)+FNN(6,7)+FNN(3,7))*GMO(7)
 Y(4)=-(FN(3)-FN(4)+FN(6)+FV*(SN1SV-2.*SN2SV)+C*(-FNN(3,3)-FNV(3)*
1(SN1SV-2.*SN2SV)+FNN(3,4)-FNN(3,6))+(ETAD-ETA)*(-.5D0*FNN(4,4)+
2.5D0*FNV(4)*(SN1SV-2.*SN2SV)+.5D0*FNN(3,4)+.5D0*FNN(4,6))+W*(
3SN1SV-2.*SN2SV)*FVV+W*(FNV(3)-FNV(4)+FNV(6)))
 X(5,1)=(.75D0*FNN(4,4)+SN1SV*((-.75D0*SN1SV+SN2SV)*FVV-.5D0*
1FNV(3)-.5D0*FNV(7)+1.5D0*FNV(1))+SN2SV*(-2.*FNV(1)+FNV(4))+
2FNN(1,3)-1.5D0*FNN(1,4)+FNN(1,7)-.5D0*FNN(3,4)-.5D0*FNN(4,7))*
3GMO(1)
 X(5,2)=(FNN(3,3)+.75D0*FNN(4,4)+(.5D0*SN1SV-2.*SN2SV)*(1.5D0*
1SN1SV-2.*SN2SV)*FVV+SN1SV*(2.*FNV(3)-1.5D0*FNV(4)+1.5D0*FNV(2)+
2.5D0*FNV(7))+SN2SV*(-4.*FNV(3)+4.*FNV(4)-2.*FNV(7)-2.*FNV(2))+
3FNN(2,3)-1.5D0*FNN(2,4)+FNN(2,7)-2.*FNN(3,4)-.5D0*FNN(4,7)+
4FNN(3,7))*GMO(2)
 X(5,3)=(-FNN(3,3)+.75D0*FNN(4,4)+SN1SV*((.75D0*SN1SV-SN2SV)*FVV+
11.5D0*FNV(5)-FNV(3)-1.5D0*FNV(4)+.5D0*FNV(7))+SN2SV*(2.*FNV(3)-2.
2*FNV(5)+FNV(4))+FNN(3,4)+FNN(3,5)-1.5D0*FNN(4,5)-.5D0*FNN(4,7)+
3FNN(5,7)-FNN(3,7))*GMO(5)
 X(5,4)=(FNN(3,3)+1.5D0*FNN(4,4)+(SN1SV-2.*SN2SV)*(1.5D0*SN1SV-2.*
1SN2SV)*FVV+SN1SV*(1.5D0*FNV(6)-3.*FMV(4)+2.5D0*FNV(3)+FNV(7))+
2SN2SV*(-4.*FNV(3)+5.*FNV(4)-2.*FNV(6)-2.*FNV(7))-2.5D0*FNN(3,4)+
3FNN(3,6)-1.5D0*FNN(4,6)-FNN(4,7)+FNN(6,7)+FNN(3,7))*GMO(6)
 X(5,5)=(FNN(3,3)+2.25D0*FNN(4,4)+FNN(7,7)+(1.5D0*SN1SV-2.*SN2SV)*
1*2*FVV+(3.*SN1SV-4.*SN2SV)*(FNV(3)+FNV(7)-1.5D0*FNV(4))-3.*
2FNN(3,4)-3.*FNN(4,7)+2.*FNN(3,7))*GMO(7)
 Y(5)=-(FN(3)-1.5D0*FN(4)+FN(7)+FV*(1.5D0*SN1SV-2.*SN2SV)+C*(-
1FNN(3,3)-(1.5D0*SN1SV-2.*SN2SV)*FNV(3)-FNN(3,7)+1.5D0*FNN(3,4))+
2(ETAD-ETA)*(-.75D0*FNN(4,4)+(.75D0*SN1SV-SN2SV)*FNV(4)+.5D0*
3FNN(3,4)+.5D0*FNN(4,7))+W*(1.5D0*SN1SV-2.*SN2SV)*FVV+W*(FNV(7)
4+FNV(3)-1.5D0*FNV(4)))
 DEBUG ((X(I,J),J=1,5),I=1,5)
 DEBUG (Y(I),I=1,5)
 RETURN
 END
```

```
$IBFTC LBINT
C SUBPROGRAM FOR 4 PUINT INTERPOLATION
C
C THIS SUBPROGRAM PERFORMS 4-POINT INTERPOLATION BY THE METHOD OF
C LAGRANGE. X AND Y ARE THE INDEPENDENT AND DEPENDENT VARIABLES,
C RESPECTIVELY, IN A TABLE OF N ENTRIES. Z IS THE VALUE OF X DESIRED.
C BINT IS THE INTERPOLATED VALUE OF Y.
      FUNCTION BINT(X,Y,Z,N)
      DIMENSION X(67),Y(67)
      M1=1
      M2=N
    5 IF(M2-M1-1)7,7,6
    6 MTEM=M1+INT(.5*(FLOAT(M2-M1)+.0001))
      IF(Z-X(MTEM))8,1,9
    8 M2=MTEM
      GO TO 5
    9 M1=MTEM
      GO TO 5
    1 BINT=Y(MTEM)
      RETURN
    7 IF(M1-1)2,2,3
    2 I=2
      GO TO 4
    3 IF(M2-N)11,10,10
   10 I=N-2
      GO TO 4
   11 I=M1
    4 Q1=Z-X(I-1)
      Q2=Z-X(I)
      Q3=Z-X(I+1)
      Q4=Z-X(I+2)
      Q12=Q1*Q2
      Q34=Q3*Q4
      P21=X(I)-X(I-1)
      P32=X(I+1)-X(I)
      P42=X(I+2)-X(I)
      P31=X(I+1)-X(I-1)
      P41=X(I+2)-X(I-1)
      P43=X(I+2)-X(I+1)
      BINT=Q34*(Q1*Y(I)/(P32*P42)-Q2*Y(I-1)/(P31*P41))/P21+Q12*(Q3*Y(I+2
     1)/(P41*P42)-Q4*Y(I+1)/(P31*P32))/P43
      RETURN
      END
```

```
$IBFTC LEXPC
C SUBPROGRAM FOR ANTICIPATING AND PREVENTING POSSIBLE UNDERFLOWS
C
C THIS SUBPROGRAM SETS EXPONENTIALS EQUAL TO 0 IF THEIR ARGUMENT IS
C SMALLER THAN -72.
      FUNCTION EXPC(A)
    2 IF(A+72.)3,4,4
    3 EXPC=0.
      GO TO 5
    4 EXPC=EXP(A)
    5 RETURN
      END
```

```
$IBFTC LINV
C SUBPROGRAM FOR INVERTING A 5X5 MATRIX
C
C THIS SUBPROGRAM INVERTS A MATRIX BY THE METHOD OF CROUT. THE ELEMENTS
C ARE NOT REARRANGED. THE DIAGONAL MAY HAVE NO ZERO ELEMENTS. THE MATRIX
C IS ASSUMED TO BE STORED IN REGION AA. THE INVERSE IS STORED IN THE
C SQUARE SUBARRAY A(1,6) THROUGH A(5,10).
      SUBROUTINE INVERT(AA,A)
      DOUBLE PRECISION A(5,11),AA(5,5),SUM
      MAG=5
      BIG = 1.1
      SMAL = 0.9
      L1=MAG+1
      L2=2*MAG
      L3=L2+1
      L4=MAG-1
C SAVE MATRIX AND AUGMENT MATRIX.
 101  DO 1003 I1=1,MAG
 102  DO 1001 J1=L1,L3
 1001 A(I1,J1) = 0.0
 103  DO 1002 J2=1,MAG
      A(I1,J2)=AA(I1,J2)
 1002 A(I1,L3)=A(I1,L3)+A(I1,J2)
      A(I1,L3)=A(I1,L3)+1.0
      J3=I1+MAG
      A(I1,J3)=1.0
 1003 CONTINUE
C BEGIN FORWARD SOLUTION.
 201  DO 2001 J4=2,L3
 2001 A(1,J4)=A(1,J4)/A(1,1)
      LORA=2
 2002 LOR1=LORA-1
      LOR2=LORA+1
 202  DO 2003 I2=LORA,MAG
 203  DO 2003 K1=1,LOR1
 2003 A(I2,LORA)=A(I2,LORA)-A(I2,K1)*A(K1,LORA)
 204  DO 2005 J5=LOR2,L3
      SUM = 0.0
 205  DO 2004 K2=1,LOR1
 2004 SUM=SUM+A(LORA,K2)*A(K2,J5)
 2005 A(LORA,J5)=(A(LORA,J5)-SUM)/A(LORA,LORA)
      IF(MAG-LORA)999,401,999
  999 LORA = LORA+1
      GO TO 2002
C BEGIN BACK SOLUTION.
 401  DO 4001 N2=1,L4
      I4=MAG-N2
 402  DO 4001 J7=L1,L3
 403  DO 4001 KSUM=1,N2
      K3=L1-KSUM
      A(I4,J7)=A(I4,J7)-A(I4,K3)*A(K3,J7)
```

```
 4001 CONTINUE
10000 RETURN
      END
```

APPENDIX C

CUTOFF OF H AND H_2 PARTITION FUNCTIONS

If the energies of the excited electronic states of H and H_2 were calculated considering all neighboring particles, there would probably be a finite number of bound states; therefore, no difficulty would arise in evaluating the partition functions. Unfortunately, no rational experimentally verified method has been developed for calculating these perturbed energy levels for conditions in this report, and in most cases the perturbations caused by the neighboring free particles are small (ref. 10). Consequently, it is customary to use the unperturbed energy levels (or term values) and to cutoff the series in the partition function at some reasonable energy level to prevent the series from diverging to infinity.

Cox (ref. 35) has pointed out that for high degrees of ionization the perturbation of the energy levels is due principally to coulomb forces, so that one method of cutoff should be used, whereas for low degrees of ionization the perturbation of the energy levels is due principally to neutral particles, so that another method of cutoff should be used. In this report the two methods used were the Debye-Hückel cutoff and a modification of the Bethe cutoff (ref. 36). The versions of these two cutoffs used herein are discussed in the following paragraphs.

In the Debye-Hückel cutoff (ref. 10) states are not counted in the partition function if their unperturbed ionization energy is less than the absolute value of the lowering of the ionization potential ΔI, which is given by (ref. 34)

$$\Delta I = \frac{Ze^2}{4\pi hc\epsilon_o}\left(\frac{e^2}{\epsilon_o kT}\sum_i z_i^2\hat{N}_i\right)^{1/2} \tag{C1}$$

Here the summation is over all species.

For hydrogen atoms, strict adherence to this cutoff results in large discontinuities in the partition function as the charged-particle density is varied at high temperatures. This can cause serious difficulties in numerical methods for finding equilibrium and is physically unrealistic because states near the cutoff are greatly broadened. A more realistic approach is to cut off each state gradually. In this report this gradual cutoff is accomplished by essentially the same method used by Krascella (ref. 1). Let F_n be the fraction of the contribution of the unperturbed state to the divergent partition function to be counted in the cutoff partition function. Then

$$\left.\begin{array}{ll}
F_n = 1 & \left(\dfrac{I_n + I_{n+1}}{2} - \Delta I \geq 0\right) \\[2ex]
F_n = \dfrac{I_n - \Delta I}{I_n - I_{n+1}} + \dfrac{1}{2} & \left(\begin{array}{l} \dfrac{I_n + I_{n+1}}{2} - \Delta I < 0 \\ \text{and} \\ I_n - \Delta I \geq 0 \end{array}\right) \\[6ex]
F_n = \dfrac{I_n - \Delta I}{I_{n-1} - I_n} + \dfrac{1}{2} & \left(\begin{array}{l} I_n - \Delta I < 0 \\ \text{and} \\ \Delta I - \dfrac{I_{n-1} + I_n}{2} < 0 \end{array}\right) \\[6ex]
F_n = 0 & \left(\Delta I - \dfrac{I_{n-1} + I_n}{2} \geq 0\right)
\end{array}\right\} \qquad \text{(C2)}$$

where I_{n-1}, I_n, and I_{n+1} are all for the same Rydberg series. (If the $n - 1$ state did not exist, a weighted average of the I_{n-1} for Rydberg series that did exist was used.) To summarize equation (C2) (1) if ΔI was less than $(I_n + I_{n+1})/2$, there was no cutoff; (2) if ΔI equaled I_n the state was half cut off; (3) if ΔI was greater than $(I_{n-1} + I_n)/2$, the state was completely cut off; and (4) for intermediate values of ΔI, the cutoff was linear in ΔI.

In the original Bethe cutoff (ref. 36), all states were cut off whose highly excited electron had a radius a_n greater than half the average distance between neighboring molecules. This half distance r_o was taken as the radius of a sphere whose volume was equal to the gas volume per molecule. The radius a_n was given by

$$a_n = a_o n^2 \qquad \text{(C3)}$$

This cutoff was used by Olsen (ref. 37). A modified Bethe cutoff with the cutoff accomplished gradually in a manner linear in n was used by Bond (ref. 38) and Pike (ref. 39).

Equation (C3) is realistic for H atoms. However, for H_2^*, a more realistic approximation was made. For Rydberg atomic orbitals of an atom

$$a_n \approx a_o(n^+)^2 = a_o \frac{R_y}{I_e} \tag{C4}$$

(ref. 40) where I_e should be the average value for the singlet and triplet states if a ^2S core is present. Equation (C4) is also valid for diatomic molecules (such as H_2^*) with a $^2\Sigma$ core (ref. 40) and was used for H_2^* in this report. For a hydrogen plasma the half distance r_o is

$$r_o = \left[\frac{3}{4\pi(\hat{N}_1 + \hat{N}_2 + \hat{N}_4 + \hat{N}_5 + \hat{N}_6 + \hat{N}_7)}\right]^{1/3} \tag{C5}$$

The equations for F_n for the modified Bethe cutoff were obtained by replacing I_{n-1}, I_n, I_{n+1}, and ΔI in equation (C2) by $-a_{n-1}^{1/2}$, $-a_n^{1/2}$, $-a_{n+1}^{1/2}$, and $-r_o^{1/2}$, respectively. Thus, for H atoms F_n was the same as in the Bond modification (ref. 38) to the Bethe cutoff.

In computing q_1 and q_4', F_n was calculated for each state by both the Debye-Hückel cutoff and the modified Bethe cutoff, and the smaller value was used. Hence, for low degrees of ionization the Bethe cutoff was always effective. At high degrees of ionization the method of cutoff depended on the conditions, and no general statement can be made.

APPENDIX D

METHODS OF OBTAINING CONSTANTS OF EXCITED ELECTRONIC STATES H_2^*

For all excited Rydberg states H_2^*, Hund's coupling case (b) (refs. 17 and 20) was assumed to hold. For each Rydberg state, a Morse potential (ref. 17) was used as a model to calculate the partition function. The formula for a Morse potential is

$$U(r) = \widetilde{T} + D\left[1 - e^{-\beta(r-r_e)}\right]^2 \tag{D1}$$

The vibrational term values $T^+ + G_v$ (see fig. 8) of Morse oscillator are (ref. 17, p. 101)

$$T^+ + G_v = \widetilde{T} + \beta\left(\frac{Dh}{2\pi^2 c\mu}\right)^{1/2}\left(v + \frac{1}{2}\right) - \frac{h\beta^2}{8\pi^2 c\mu}\left(v + \frac{1}{2}\right)^2 \tag{D2}$$

measured from the rotationless ground vibrational state of H_2. If

$$\omega \equiv \beta\left(\frac{Dh}{2\pi^2 c\mu}\right)^{1/2} \tag{D3}$$

equation (D2) becomes

$$T^+ + G_v = \widetilde{T} + \omega\left(v + \frac{1}{2}\right) - \frac{\omega^2}{4D}\left(v + \frac{1}{2}\right)^2 \tag{D4}$$

For electronic states with no hump in their potentials (see lower H_2^* potential in fig. 8) and known vibrational term values, the appropriate method of fitting the Morse potential to the actual potential has been given in reference 18. It includes making W for the Morse potential the same as the actual W, where W for these states is the energy difference between the dissociation asymptote and the rotationless ground vibrational level of the state (see fig. 8). From equation (D4)

$$D = \frac{W + \frac{\omega}{2} + \sqrt{W(W + \omega)}}{2} \tag{D5}$$

The constant ω was determined by fitting the excited vibrational energy levels (ref. 18).

In general, D for the Morse potential was not the same as the actual well depth, and to determine it a knowledge of the actual dissociation asymptote was, of course, required.

As shown in figure 8, the potential curves of some excited electronic states H_2^* possess a hump, which presented a problem because the Morse potential has no hump. However, the principal effect of the decrease in the potential energy to the right of the hump is to broaden those bound energy levels lying above the dissociation asymptote but not shift them much. Hence, a good approximation was to set W for the Morse potential equal to the energy difference between the top of the hump and the rotationless ground vibrational state (see upper H_2^* potential in fig. 8). The Morse well depth is then given by equation (D5). A knowledge of the actual dissociation asymptote and the hump height H (if any) are required to find W and D.

For all excited electronic states of H_2 in this report, the dissociation products are the atoms H(1) and H(n), where the quantity in parentheses is the principal quantum number. The energy of the dissociation asymptote is thus determined by the value of n. The state H(n) was determined for each electronic state of H_2 by the correlation rules (ref. 17) also known as noncrossing rules. (Note that fig. 157 of ref. 17 does not apply to H_2 despite the label H_2 on it.) The values of n in H(n) are tabulated in table II (pp. 76 and 77).

Some of the hump heights of H_2^* were obtained from the literature, whereas others had to be predicted. Six electronic states H_2^* have been reported (refs. 15, 41, and 42) to possess humps, and the heights have been given. Of these, five have promoted molecular orbitals (MO). The sixth has a much smaller hump than the other five. On the other hand, two states with promoted molecular orbitals but no humps have been reported (ref. 41). Unfortunately, there are many electronic states H_2^* for which there are no reports on the presence or absence of humps. For these it was assumed that there was no hump if there was no promoted MO. For states with promoted molecular orbitals, an approximation was made. The ratios H/δ (fig. 9) were calculated for the seven electronic states with promoted molecular orbitals for which values of H were available (including the two states with $H = 0$). An average of the ratios was then calculated by using the electronic statistical weights g_e as weighting factors. This average had the value 0.15036. It was assumed that all other states with promoted molecular orbitals had $H/\delta = 0.15036$. Values of H are tabulated in table II.

It was necessary to have Morse potentials for every Rydberg state H_2^* with n of the excited electron of the molecule having values from 2 to 17. A different Morse potential was used for each electronic state with n from 2 to 4, and experimental term values were used when available in determining the Morse potential. For large n all states H_2^* have potentials nearly the same as H_2^+, and for n greater than 4 there is little experimental information. Hence, for electronic states with n from 5 to 17, the same Morse potential was used for all states with a given value of n. The constants for Morse potentials with n from 5 to 17 were estimated from the constants for H_2^+ and the averages of the constants for the $n = 3$ states. (Constants for many of the $n = 4$ states were unreliable or had to be estimated.) The most used methods of determining or estimating Morse constants for $n = 2$ to 17 are given below. Less used methods are described in footnotes in table II.

Morse potentials were most easily fit to states for which the rotationless ground vibrational term value, one or more excited pure (rotationless) vibrational term values, and several rotational term values were available. Setting v and G_v equal to 0 in equation (D4) gives

$$T^+ - \widetilde{T} = \frac{1}{2}\omega - \frac{\omega^2}{16D} \tag{D6}$$

Substituting equation (D6) into equation (D4)

$$G_v = \omega v - \frac{\omega^2}{4D} v(v + 1) \tag{D7}$$

Equation (D5) may be substituted into equation (D7) to get G_v in terms of ω, v, and W. In accordance with reference 18, ω was then varied to minimize the sum of the squares of the deviations of the calculated quantities G_v from the experimental quantities G_v. The well depth D was then found from equation (D5), and β was found from equation (D3). The last step was to find r_e. To do this, the Morse potential was expanded in powers of $(r - r_e)/r_e$ so the rotational term values f(v,k) for each vibrational level could be expressed by Dunham's formulae (ref. 43). The equilibrium internuclear distance r_e was then varied to minimize the sum of the squares of the deviations of the calculated quantities f from the experimental quantities f.

A more difficult problem was presented by electronic states for which no rotationless ground vibrational term values were known, but for which a number of vibration-rotation term values $T^+ + G_v + f$ were known for more than one value of v. An expression was derived from equation (D2) and Dunham's formulae which gave vibration-rotation term values in terms of the energy of the dissociation asymptote, the hump height, D, β, r_e, v, and K. The quantities D, β, and r_e were then simultaneously varied to minimize the sum of the squares of the deviations of the calculated term values from the experimental term values, using weighting factors. To be as nearly consistent with reference 18 as possible, each vibrational level for which any term values were available was given the same weight.

For some $n = 4$ states there was only one vibrational term value or none at all available. For such cases there is no good way to estimate β or ω. However, fair estimates were obtained by interpolation of β along a Rydberg series with H_2^+ as its limit. The interpolation was accomplished linearly between $n = 3$ and $n = \infty$ (i.e., H_2^+) in the $\beta - 1/n^5$ plane. When no $n = 3$ state of the Rydberg series existed, $\beta(n = 3)$ was taken as the average for all $n = 3$ states, using g_e as a weighting factor. In most cases, ω was then found from equation (D3).

For all states with $n = 5$ to 17, all Morse constants were estimated. First, the average I_e (fig. 8) for all $n = 3$ states was calculated, using the g_e as weighting factors. From this value the average quantum defect (ref. 40) was calculated. It was then assumed that the average quantum defect was independent of n (which is not strictly correct because the quantum defect would be expected to be independent of n only for large n along a Rydberg series). Thus, average values of I_e and, hence, $\widetilde{T}$ were calculated for $n = 5$ to 17. An average value of β was found for each value of n by interpolation, as described in the preceding paragraph. For each n, an average value of D was found from the average $\widetilde{T}$, the various dissociation asymptotes, and the various hump heights, using the g_e of the H_2^* states as weighting factors.

For some $n = 4$ states and all states with $n = 5$ to 17, it was necessary to estimate r_e. Herzberg (ref. 17, p. 456) gives the empirical relation

$$r_e^2\omega = \text{Constant} \tag{D8}$$

for electronic states of the same molecule. The extension of equation (D8) to the molecular ion resulting from removing an electron from that molecule is obvious. Many of the values of r_e for H_2^* are unreliable, so for this report equation (D8) was used in the form

$$\left(r_e^2\omega\right)_{H_2^*} = \left(r_e^2\omega\right)_{H_2^+} \tag{D9}$$

to estimate r_e for various electronic states H_2^*, where r_e and ω for H_2^+ were obtained from the results of Wind (refs. 21 and 44).

All values of D, β, r_e, and $\widetilde{T}$ are tabulated in table II (p. 76). In addition to D, β, r_e, and $\widetilde{T}$, equations (17) and (18) also require values of the fundamental frequency of vibration ω' (fig. 8). From equation (D4)

$$\omega' = \omega\left(1 - \frac{\omega}{2D}\right) \tag{D10}$$

This completes the determination of the constants of Rydberg states of H_2^*.

APPENDIX E

SOURCES OF EXPERIMENTAL ENERGY LEVELS OF EXCITED ELECTRONIC STATES OF H_2 AND CORRECTIONS TO THEM

The energy levels (or term values) of states of H_2^* have been determined from spectroscopic observations by a large number of investigators, but much of the early work is inaccurate. Spindler (ref. 14) took statistically weighted averages of all experimentally determined spectroscopic constants for the $1s\sigma 2p\sigma\ {}^1\Sigma$, $1s\sigma 3p\sigma\ {}^1\Sigma$, $1s\sigma 2p\pi\ {}^1\Pi$, and $1s\sigma 3p\pi\ {}^1\Pi$ states, and his values were used for vibrational term value differences (no rotation) and for equilibrium internuclear distance r_e for these four states (see table I (p. 75)). For all states it is necessary to know the absolute value of at least one term value in addition to the term value differences. The absolute values are usually measured from the rotationless ground vibrational state of $H_2^{\ddagger}$. An absolute term value for each of the four previously mentioned states was taken from the latest measurements (refs. 22, 45, and 46) (see table I). For other states all experimental data were taken only from the latest measurements (refs. 33, 47, and 48).

Although for many states Dieke (ref. 33) had the most reliable term value differences, some corrections to his absolute term values were necessary because he relied on old, far ultraviolet measurements for the absolute term values of excited singlet states and found the relative position of excited singlet states and triplet states by extrapolation to the limits of Rydberg series. However, visible, infrared, or near ultraviolet line positions were accurately measured by Dieke to determine the term values of all excited singlet states relative to each other and of all triplet states relative to each other. Consequently, Dieke's term values are accurate to within an additive constant for excited singlets and to within a different additive constant for triplets.

Field, Somerville, and Dressler (ref. 49) have examined the latest far ultraviolet measurements on singlet states (refs. 22, 45, 48, 50, and 51) and concluded that 700 meters^{-1} should be added to Dieke's term values for excited singlets, which was done in this report (see table I).

Determination of the correction to Dieke's term values for triplet states was more complicated because there are no spectral lines connecting singlet and triplet states. Kolos (ref. 52) states that Professor R. S. Mulliken believed a correction was necessary, and Kolos determined the correction by calculations from first principles. In this report reliance was put more on experimental observations, although Wind's very reliable H_2^+ term values and dissociation energy (ref. 21) based on calculations from first principles had to be used also. The derivation follows that of Beutler and Jünger (ref. 53) with two exceptions (1) the energies of all H and H_2^+ states are assumed to be known exactly relative to the rotationless ground vibrational state of $H_2^{\ddagger}$ by means of the dissociation energy of $H_2^{\ddagger}$ (table III, p. 78), the term values and ionization potential of H (ref. 54), and the term values and dissociation energy of H_2^+ (ref. 21); and (2) the relative positions of all triplet levels are known as a result of infrared measurements (refs. 33 and 55).

Observations (refs. 56 and 57) of the lines of three electronic transitions were used to draw the following conclusions:

(1) From the transition $1s\sigma 3p\pi\ {}^3\Pi \rightarrow 1s\sigma 2s\sigma\ {}^3\Sigma$ it was concluded that $1s\sigma 3p\pi\ {}^3\Pi$ ($v = 3$, $K = 3$, para) does not predissociate into H(1) + H(2), where the numbers in parentheses following each H are principal quantum numbers.

(2) From the same transition it was concluded that $1s\sigma 3p\pi\ {}^3\Pi$ ($v = 3$, $K = 4$, ortho) does predissociate into H(1) + H(2).

(3) From the transition $1s\sigma 3p\pi\ {}^3\Pi \rightarrow 1s\sigma 2s\sigma\ {}^3\Sigma$ it was concluded that $1s\sigma 3p\pi\ {}^3\Pi$ ($v = 7$, $K = 2$, para) preionizes to H_2^+ ($v = 0$, $K = 0$) + e^-.

(4) From the same transition it was concluded that $1s\sigma 3p\pi\ {}^3\Pi$ ($v = 6$, $K = 3$, ortho) does not preionize to H_2^+ ($v = 0$, $K = 1$) + e^-.

(5) From the transition $1s\sigma 3s\sigma\ {}^3\Sigma \rightarrow 1s\sigma 2p\pi\ {}^3\Pi$ it was concluded that $1s\sigma 3s\sigma\ {}^3\Sigma$ ($v = 3$, $K = 1$, ortho) does not predissociate to H(1) + H(2).

(6) From the same transition it was concluded that $1s\sigma 3s\sigma\ {}^3\Sigma$ ($v = 3$, $K = 2$, ortho) does predissociate to H(1) + H(2).

(7) From the transition $1s\sigma 4d\delta\ {}^3\Delta \rightarrow 1s\sigma 2p\pi\ {}^3\Pi$ it was concluded that $1s\sigma 4d\delta\ {}^3\Delta$ ($v = 3$, $K = 4$, para) does not preionize to H_2^+ ($v = 0$, $K = 2$) + e^-.

(8) From the same transition it was concluded that $1s\sigma 4d\delta\ {}^3\Delta$ ($v = 3$, $K = 5$, ortho) does preionize to H_2^+ ($v = 0$, $K = 3$) + e^-.

Let d be the correction to be added to Dieke's triplet term values (ref. 33). Then, from Dieke's term values, supplemented where necessary by term differences from reference 56 or estimates of term differences from reference 53, and from conclusions (1) to (8) it follows that

$$11\ 850\ 900 + d < 11\ 837\ 270\ \mathrm{m}^{-1} \tag{E1}$$

$$11\ 870\ 940 + d > 11\ 837\ 270\ \mathrm{m}^{-1} \tag{E2}$$

$$12\ 514\ 840 + d > 12\ 441\ 300\ \mathrm{m}^{-1} \tag{E3}$$

$$12\ 374\ 420 + d < 12\ 447\ 120\ \mathrm{m}^{-1} \tag{E4}$$

$$11\ 851\ 770 + d < 11\ 837\ 270\ \mathrm{m}^{-1} \tag{E5}$$

$$11\ 862\ 270 + d > 11\ 837\ 270\ \mathrm{m}^{-1} \tag{E6}$$

$$12\ 481\ 360 + d < 12\ 458\ 720\ \mathrm{m}^{-1} \tag{E7}$$

$$12\ 516\ 970 + d > 12\ 476\ 010\ \mathrm{m}^{-1} \tag{E8}$$

respectively. From equations (E1) to (E8)

$$d = -23\ 820 \pm 1180\ \mathrm{m}^{-1} \tag{E9}$$

Hence, 23 820 meter^{-1} was subtracted from each of Dieke's triplet term values (see table I, p. 75). This puts $1s\sigma 2p\pi\ {}^3\Pi$ within 760 meter^{-1} of the term values relative to H_2^+ calculated by Beutler and Jünger (ref. 53) and within 1460 meter^{-1} of the term values relative to H_2^+ calculated by Richardson (ref. 56). Beutler and Jünger and also Richardson had available less complete, less accurate data and calculations from first principles than were available for the present study.

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TABLE I. - REFERENCES FOR EXPERIMENTAL TERM VALUES OF EXCITED ELECTRONIC STATES H_2^* AND CORRECTIONS TO THEM

Excited electronic state		Reference for vibrational term value differences (no rotation)	Reference for vibration-rotation term value differences or r_e	Reference for absolute term values[a]	Amount added to absolute term values obtained from reference in preceding column,[b] m^{-1}
Term symbol	Small-internuclear-distance designation				
$^1\Sigma$	1sσ2sσ	33	33	33	700
	1sσ3sσ	33	33	33	700
$^1\Sigma$	1sσ2pσ	14	14	22	0
	1sσ3pσ	14	14	45	0
	1sσ4pσ	47	47	47	0
$^1\Pi$	1sσ2pπ	[c]14	14	46	0
	1sσ3pπ	[c]14	14	45	0
	1sσ4pπ	[c]48	47	48	0
$^1\Sigma$	1sσ3dσ	33	33	33	700
	1sσ4dσ	(d)	33	33	700
$^1\Pi$	1sσ3dπ	(c)	33	33	700
	1sσ4dπ	(c)	33	33	700
$^1\Delta$	1sσ3dδ	(c)	33	33	700
	1sσ4dδ	(c)	33	33	700
$^3\Sigma$	1sσ2sσ	33	33	33	-23 820
	1sσ3sσ	33	33	33	-23 820
$^3\Sigma$	1sσ3pσ	33	33	33	-23 820
	1sσ4pσ	33	33	33	-23 820
$^3\Pi$	1sσ2pπ	(c)	33	33	-23 820
	1sσ3pπ	(c)	33	33	-23 820
	1sσ4pπ	(c)	33	33	-23 820
$^3\Sigma$	1sσ3dσ	33	33	33	-23 820
	1sσ4dσ	33	33	33	-23 820
$^3\Pi$	1sσ3dπ	(c)	33	33	-23 820
	1sσ4dπ	(c)	33	33	-23 820
$^3\Delta$	1sσ3dδ	(c)	33	33	-23 820
	1sσ4dδ	(c)	33	33	-23 820

[a] Measured from rotationless ground vibrational state (1sσ1sσ $^1\Sigma$) of H_2.

[b] See appendix E for explanation.

[c] Virtual levels.

[d] Not given.

TABLE II. - CONSTANTS AND SUBSCRIPTS OF EXCITED ELECTRONIC STATES H_2^*

Excited electronic state		Electronic degeneracy, g_e	Principal quantum number n of excited dissociated atom[a]	Hump height, H, m^{-1}	Well depth, D, m^{-1}	Morse parameter, β, m^{-1}	Equilibrium internuclear distance, r_e, m	Energy relative to electronic ground state, $\widetilde{T}$, m^{-1}	Subscripts in computer program
Term symbol	Small-internuclear-distance designation								
$^{1}\Sigma$	1sσ2sσ	1	2	[b]0	2.0391×10^{6}	1.4529×10^{10}	1.0334×10^{-10}	9.79815×10^{6}	2, 1
	1sσ3sσ	1	3	[b]0	2.1821	1.3907	1.1181	11.17846	3, 1
	1sσ4sσ	1	3	[c]80 170	1.6923	[d]1.3448	[e]1.1290	[f]11.74843	4, 1
$^{1}\Sigma$	1sσ2pσ	1	2	[g]0	2.8848×10^{6}	0.6948×10^{10}	1.2907×10^{-10}	8.95248×10^{6}	2, 2
	1sσ3pσ	1	2	[b]0	.8796	1.7070	1.1270	10.95767	3, 2
	1sσ4pσ	1	3	[c]80 170	1.8591	1.3750	1.111	11.58169	4, 2
$^{1}\Pi$	1sσ2pπ	2	2	[h]10 550	2.0653×10^{6}	1.5493×10^{10}	1.0316×10^{-10}	9.78257×10^{6}	2, 3
	1sσ3pπ	2	3	[b]0	2.1907	1.3895	1.0440	11.16987	3, 3
	1sσ4pπ	2	4	[i]0	2.2249	1.3451	1.0555	11.66884	4, 3
$^{1}\Sigma$	1sσ3dσ	1	2	[b]241 970	1.0272×10^{6}	2.2770×10^{10}	[j]1.0740×10^{-10}	11.05203×10^{6}	2, 4
	1sσ4dσ	1	3	[c]80 170	1.8310	[d]1.5551	1.4205	11.60980	3, 4
$^{1}\Pi$	1sσ3dπ	2	2	[b]241 970	1.0053×10^{6}	2.2658×10^{10}	1.1639×10^{-10}	11.07394×10^{6}	2, 5
	1sσ4dπ	2	3	[c]80 170	1.7965	1.4662	1.3972	11.64430	3, 5
$^{1}\Delta$	1sσ3dδ	2	3	[b]0	2.2368×10^{6}	1.3204×10^{10}	0.9916×10^{-10}	11.12376×10^{6}	2, 6
	1sσ4dδ	2	4	[k]0	2.2431	[d]1.3281	.8959	11.65069	3, 6
$^{1}\Sigma$	1sσ4fσ	1	3	[c]80 170	1.8416×10^{6}	[l]1.4068×10^{10}	[e]1.0809×10^{-10}	[m]11.59920×10^{6}	2, 7
$^{1}\Pi$	1sσ4fπ	2	3	[i]73 600	[i]1.7686×10^{6}	[i]1.6348×10^{10}	[i]1.0583×10^{-10}	[i]11.66560×10^{6}	2, 8
$^{1}\Delta$	1sσ4fδ	2	3	[c]80 170	1.8327×10^{6}	[l]1.4068×10^{10}	[e]1.0821×10^{-10}	[m]11.60810×10^{6}	2, 9
$^{1}\varphi$	1sσ4fφ	2	4	[k]0	2.2751×10^{6}	[l]1.4068×10^{10}	[e]1.0253×10^{-10}	[m]11.61865×10^{6}	2, 10
$^{3}\Sigma$	1sσ2sσ	3	2	[b]0	2.4716×10^{6}	1.4844×10^{10}	0.9955×10^{-10}	9.36566×10^{6}	2, 11
	1sσ3sσ	3	3	[b]0	2.3004	1.3641	1.0613	11.06023	3, 11
	1sσ4sσ	3	3	[c]80 170	1.8086	[d]1.3385	[e]1.1132	[n]11.63219	4, 11
$^{3}\Sigma$	1sσ3pσ	3	2	[b]0	1.2957×10^{6}	1.8309×10^{10}	1.0869×10^{-10}	10.54161×10^{6}	2, 12
	1sσ4pσ	3	2	[c]309 210	.7202	2.6694	1.0654	11.42631	3, 12
$^{3}\Pi$	1sσ2pπ	6	2	[b]0	2.4785×10^{6}	1.3497×10^{10}	1.0499×10^{-10}	9.35873×10^{6}	2, 13
	1sσ3pπ	6	3	[b]0	2.3161	1.3407	1.0667	11.04446	3, 13
	1sσ4pπ	6	3	[c]80 170	1.8545	1.6084	1.0603	11.58621	4, 13

[a] Excited electronic states of H_2 in this table dissociate to one ground state $H^\ddagger$ atom and one excited H^* atom.

[b] Ref. 41.

[c] Calculated assuming $H/\delta = 0.15036$.

[d] Interpolated between n = 3 and H_2^+ along Rydberg series.

[e] Assumed value of ωr_e^2 same as for H_2^+.

[f] Ref. 58.

[g] Ref. 59.

[h] Ref. 15.

[i] Energy levels, hump height, and r_e from ref. 42.

[j] Irregular term values; thus, r_e determined by method on p. 112 of ref. 56.

[k] Assumed value of 0 because of unpromoted MO.

[l] Interpolated between n = 3 (average for all states) and H_2^+.

[m] Estimated.

[n] Ref. 60.

TABLE II. - Concluded. CONSTANTS AND SUBSCRIPTS OF EXCITED ELECTRONIC STATES H_2^*

Excited electronic state		Electronic degeneracy, g_e	Principal quantum number n of excited dissociated atom[a]	Hump height, H, m^{-1}	Well depth, D, m^{-1}	Morse parameter, β, m^{-1}	Equilibrium internuclear distance, r_e, m	Energy relative to electronic ground state, $\tilde{T}$, m^{-1}	Subscripts in computer program
Term symbol	Small-internuclear-distance designation								
$^3\Sigma$	1sσ3dσ	3	2	[b]330 700	1.1139×10^6	1.9680×10^{10}	1.4461×10^{-10}	11.05411×10^6	2, 14
	1sσ4dσ	3	3	[c]80 170	1.8156	1.4693	[j].9298	11.62514	3, 14
$^3\Pi$	1sσ3dπ	6	2	[b]330 700	1.1000×10^6	2.1220×10^{10}	1.1466×10^{-10}	11.06801×10^6	2, 15
	1sσ4dπ	6	3	[c]80 170	1.8129	1.5022	1.1675	11.62789	3, 15
$^3\Delta$	1sσ3dδ	6	3	[b]0	2.2430×10^6	1.3103×10^{10}	0.9937×10^{-10}	11.11759×10^6	2, 16
	1sσ4dδ	6	4	[k]0	2.2575	1.3086	.8348	11.63629	3, 16
$^3\Sigma$	1sσ4fσ	3	3	[c]80 170	1.8037×10^6	[l]1.4068×10^{10}	[e]1.0866×10^{-10}	[n]11.63704×10^6	2, 17
$^3\Pi$	1sσ4fπ	6	4	[k]0	2.2551×10^6	[l]1.4068×10^{10}	[e]1.0276×10^{-10}	[n]11.63865×10^6	2, 18
$^3\Delta$	1sσ4fδ	6	3	[c]80 170	1.8327×10^6	[l]1.4068×10^{10}	[e]1.0821×10^{-10}	[m]11.60804×10^6	2, 19
$^3\varphi$	1sσ4fφ	6	4	[k]0	2.2752×10^6	[l]1.4068×10^{10}	[e]1.0253×10^{-10}	[m]11.61859×10^6	2, 20
Various	1sσ5	100	3 to 5	Various	2.0408×10^6	[l]1.3556×10^{10}	[e]1.0732×10^{-10}	11.87246×10^6	2, 21
	1sσ6	144	4 to 6		2.1083	[l]1.3406	[e]1.0703	12.01307	3, 21
	1sσ7	196	4 to 7		2.1482	[l]1.3352	[e]1.0676	12.09721	4, 21
	1sσ8	256	5 to 8		2.1710	[l]1.3330	[e]1.0657	12.15153	5, 21
	1sσ9	324	6 to 9		2.1878	[l]1.3319	[e]1.0641	12.18862	6, 21
Various	1sσ10	400	6 to 10	Various	2.2005×10^6	[l]1.3314×10^{10}	[e]1.0628×10^{-10}	12.21506×10^6	2, 22
	1sσ11	484	7 to 11		2.2091	[l]1.3311	[e]1.0617	12.23457	3, 22
	1sσ12	576	8 to 12		2.2159	[l]1.3309	[e]1.0610	12.24938	4, 22
	1sσ13	676	9 to 13		2.2214	[l]1.3308	[e]1.0605	12.26088	5, 22
	1sσ14	784	9 to 14		2.2258	[l]1.3307	[e]1.0600	12.27000	6, 22
Various	1sσ15	900	10 to 15	Various	2.2291×10^6	[l]1.3307×10^{10}	[e]1.0595×10^{-10}	12.27734×10^6	2, 23
	1sσ16	1024	11 to 16		2.2319	[l]1.3307	[e]1.0592	12.28335	3, 23
	1sσ17	1156	11 to 17		2.2343	[l]1.3307	[e]1.0589	12.28832	4, 23

[b] Ref. 41.

[c] Calculated assuming H/δ = 0.15036.

[e] Assumed value of ωr_e^2 same as for H_2^+.

[j] Irregular term values, thus, R_e determined by method on p. 112 of ref. 56.

[k] Assumed value of 0 because of unpromoted MO.

[l] Interpolated between n = 3 (average for all states) and H_2^+.

[m] Estimated.

[n] Ref. 60.

TABLE III. - DISSOCIATION, PHOTODETACHMENT, AND IONIZATION ENERGIES

Reaction[a]	Energy absorbed in reaction,[b] m^{-1}	Reference
$H_2^{\ddagger}\ (1s\sigma 1s\sigma\ {}^1\Sigma) \rightarrow 2H^{\ddagger}$	$W_4^{\ddagger} = 3.61136\times10^6$	46, 61
$H_2^{+}\ (1s\sigma\ {}^2\Sigma) \rightarrow H^{\ddagger} + H^{+}$	$W_6 = 2.13794\times10^6$	21
$H_3^{+}\ ({}^1A_1) \rightarrow 2H^{\ddagger} + H^{+}$	$W_7 = 7.2707\times10^6$	13
$H^{-} \rightarrow H^{\ddagger} + e^{-}$	$I_5 = 6.2187\times10^5$	62
$H^{\ddagger} \rightarrow H^{+} + e^{-}$	$I_1^{\ddagger} = 1.096788\times10^7$	54

[a] Molecules and molecular ions are assumed to be in their rotationless ground vibrational states.

[b] All values given are differences in term values (energy/hc) of reactants and products; hence, units are m^{-1}

TABLE IV. - ROTATIONAL TERM VALUES OF GROUND ELECTRONIC STATE ($1s\sigma 1s\sigma\ ^1\Sigma$) OF H_2

Total angular momentum quantum number, J	Vibrational quantum number, v														
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
	Rotational term value, f, m^{-1}														
0	0.	0.	-0.	-0.	-0.	0.	0.	-0.	0.	-0.	-0.	0.	-0.	-0.	0.
1	11852.	11257.	10679.	10111.	9565.	8988.	8413.	7821.	7211.	6557.	5849.	5068.	4152.	3079.	1727.
2	35453.	33672.	31932.	30233.	28582.	26865.	25136.	23363.	21527.	19579.	17463.	15123.	12365.	9114.	4994.
3	70587.	67029.	63564.	60171.	56881.	53456.	50009.	46467.	42801.	38910.	34663.	29976.	24489.	17879.	9439.
4	116932.	111037.	105286.	99643.	94162.	88500.	82760.	76875.	70757.	64279.	57196.	49365.	40218.	29090.	14500.
5	174094.	165299.	156715.	148294.	140077.	131651.	123062.	114259.	105089.	95367.	84730.	72917.	59127.	42240.	
6	241600.	229358.	217404.	205686.	194196.	182501.	170530.	158230.	145398.	131803.	116864.	100218.	80722.	56691.	
7	318852.	302680.	286854.	271338.	256050.	240547.	224697.	208344.	191254.	173066.	153109.	130746.	104418.	71609.	
8	405346.	384685.	364505.	344702.	325119.	305303.	285058.	264112.	242156.	218740.	192981.	163947.	129518.	85558.	
9	500392.	474767.	449781.	425219.	400851.	376206.	351079.	325015.	297609.	268282.	235916.	199246.	155153.		
10	603335.	572282.	542057.	512290.	482679.	452715.	422177.	390486.	357056.	321116.	281300.	235841.	180225.		
11	713500.	676570.	640698.	605301.	569997.	534273.	497810.	459917.	419866.	276580.	328393.	272721.	203042.		
12	830194.	786987.	745062.	703666.	662221.	620288.	577390.	532733.	485385.	433965.	376318.	308806.			
13	952734.	902894.	854558.	806738.	758744.	710158.	660331.	608326.	553002.	492575.	424316.	342614.			
14	1080441.	1023684.	968516.	913920.	858987.	803306.	746059.	686133.	622111.	551738.	471342.	371564.			
15	1212683.	1148721.	1086399.	1024604.	962369.	899130.	833977.	765532.	691994.	610507.	515770.				
16	1348894.	1277402.	1207582.	1138229.	1068309.	997097.	923479.	845805.	761758.	667760.	555461.				
17	1488465.	1409142.	1331524.	1254241.	1176241.	1096586.	1013929.	926305.	830773.	722407.					
18	1630829.	1543379.	1457681.	1372094.	1285621.	1197038.	1104753.	1006324.	897973.	772062.					
19	1775451.	1679592.	1585510.	1491280.	1395881.	1297904.	1195296.	1084950.	961921.						
20	1921791.	1817272.	1714504.	1611313.	1506573.	1398545.	1284780.	1161330.	1020958.						
21	2069372.	1955961.	1844169.	1731686.	1617105.	1498380.	1372526.	1234226.	1070223.						
22	2217699.	2095209.	1974039.	1851871.	1726957.	1596827.	1457534.	1301644.							
23	2366299.	2234566.	2103658.	1971389.	1835555.	1693041.	1538665.	1359827.							
24	2514773.	2373579.	2232613.	2089735.	1942227.	1786214.	1614187.								
25	2662745.	2511826.	2360462.	2206391.	2046374.	1875100.	1680320.								
26	2809896.	2648894.	2486726.	2320839.	2147107.	1958130.									
27	2955879.	2784347.	2610949.	2432370.	2243405.	2031554.									
28	3100329.	2917813.	2732578.	2540291.	2333484.										
29	3242913.	3048916.	2851009.	2643523.	2414117.										
30	3383239.	3177186.	2965595.	2740537.											
31	3520920.	3302143.	3075429.	2828060.											
32	3655593.	3423200.	3179162.												
33	3786839.	3539599.	3273966.												
34	3914204.	3650081.													
35	4037023.	3752564.													
36	4154504.														
37	4265188.														
38	4364780.														

TABLE V. - NUMBER DENSITIES OF SPECIES IN HYDROGEN PLASMA[a, b]

(a) Pressure, 1.01325×10^{5} N/m^2 (1 atm)

Temperature, T, K	$H_2^{\ddagger}$	H_2^*	$H^{\ddagger}$	H^*	e^-	H^-	H_3^+	H_2^+	H^+
	[c]Number density, $\hat{N}_i$, m^{-3}								
300	2.447E 25	0.	1.030E-10	0.	0.	0.	0.	0.	0.
400	1.835E 25	0.	2.449E-01	0.	0.	0.	0.	0.	0.
500	1.468E 25	0.	1.021E 05	0.	0.	0.	0.	0.	0.
600	1.223E 25	0.	5.647E 08	0.	0.	0.	0.	0.	0.
700	1.049E 25	0.	2.646E 11	0.	0.	0.	0.	0.	0.
800	9.175E 24	0.	2.652E 13	0.	0.	0.	0.	0.	0.
900	8.155E 24	0.	9.508E 14	0.	0.	0.	0.	0.	0.
1000	7.340E 24	0.	1.661E 16	0.	0.	0.	0.	0.	0.
1100	6.672E 24	0.	1.720E 17	0.	0.	0.	0.	0.	0.
1200	6.116E 24	0.	1.203E 18	0.	0.	0.	0.	0.	0.
1300	5.646E 24	0.	6.225E 18	0.	0.	0.	0.	0.	0.
1400	5.243E 24	0.	2.541E 19	0.	6.863E 03	2.055E-01	6.863E 03	0.	0.
1500	4.893E 24	0.	8.583E 19	0.	1.536E 05	9.152E 00	1.536E 05	0.	0.
1600	4.587E 24	0.	2.485E 20	0.	2.331E 06	2.517E 02	2.332E 06	0.	0.
1800	4.076E 24	9.173E-07	1.455E 21	1.618E-07	2.174E 08	6.183E 04	2.174E 08	0.	0.
2000	3.664E 24	1.357E-03	5.942E 21	4.740E-04	8.196E 09	4.947E 06	8.201E 09	0.	0.
2200	3.317E 24	4.926E-01	1.867E 22	3.231E-01	1.598E 11	1.749E 08	1.599E 11	2.507E 05	2.051E 06
2400	3.010E 24	6.683E 01	4.808E 22	7.367E 01	1.894E 12	3.338E 09	1.897E 12	1.988E 07	2.003E 08
2600	2.717E 24	4.220E 03	1.059E 23	7.208E 03	1.523E 13	3.935E 10	1.525E 13	8.047E 08	9.730E 09
2800	2.416E 24	1.444E 05	2.051E 23	3.608E 05	8.955E 13	3.137E 11	8.957E 13	1.913E 10	2.734E 11
3000	2.091E 24	2.978E 06	3.557E 23	1.048E 07	4.065E 14	1.799E 12	4.031E 14	2.952E 11	4.961E 12
3200	1.735E 24	3.990E 07	5.582E 23	1.940E 08	1.485E 15	7.774E 12	1.427E 15	3.160E 12	6.287E 13
3400	1.361E 24	3.662E 08	7.981E 23	2.448E 09	4.566E 15	2.546E 13	3.985E 15	2.434E 13	5.825E 14
3600	9.950E 23	2.398E 09	1.044E 24	2.222E 10	1.257E 16	7.555E 13	8.536E 15	1.346E 14	3.974E 15
3800	6.751E 23	1.162E 10	1.256E 24	1.516E 11	3.340E 16	1.955E 14	1.347E 16	5.229E 14	1.961E 16
4000	4.283E 23	4.346E 10	1.407E 24	8.105E 11	8.836E 16	4.766E 14	1.589E 16	1.462E 15	7.149E 16
4300	1.999E 23	2.149E 11	1.507E 24	5.933E 12	3.527E 17	1.554E 15	1.435E 16	4.471E 15	3.354E 17
4600	9.143E 22	7.725E 11	1.504E 24	4.247E 13	1.205E 18	4.210E 15	1.084E 16	1.032E 16	1.188E 18
4900	4.331E 22	2.258E 12	1.455E 24	2.037E 14	3.536E 18	9.547E 15	7.835E 15	2.042E 16	3.518E 18
5200	2.173E 22	5.731E 12	1.390E 24	8.119E 14	9.143E 18	1.962E 16	5.708E 15	3.661E 16	9.120E 18
5600	9.518E 21	1.694E 13	1.301E 24	4.102E 15	2.765E 19	4.395E 16	3.885E 15	7.151E 16	2.761E 19
6000	4.598E 21	4.360E 13	1.219E 24	1.697E 16	7.213E 19	3.705E 16	2.777E 15	1.271E 17	7.209E 19
6500	2.081E 21	1.247E 14	1.127E 24	8.055E 16	2.028E 20	1.789E 17	1.942E 15	2.352E 17	2.028E 20
7000	1.047E 21	3.142E 14	1.046E 24	3.156E 17	4.926E 20	3.274E 17	1.441E 15	3.973E 17	4.926E 20
7500	5.732E 20	7.181E 14	9.759E 23	1.059E 18	1.064E 21	5.463E 17	1.122E 15	6.235E 17	1.064E 21
8000	3.362E 20	1.510E 15	9.129E 23	3.125E 18	2.090E 21	8.455E 17	9.063E 14	9.205E 17	2.090E 21
9000	1.347E 20	5.387E 15	8.025E 23	1.977E 19	6.438E 21	1.694E 18	5.390E 14	1.727E 18	6.438E 21
10000	6.156E 19	1.489E 16	7.025E 23	8.853E 19	1.575E 22	2.305E 18	4.729E 14	2.745E 18	1.575E 22
11000	2.987E 19	3.267E 16	6.029E 23	3.009E 20	3.227E 22	3.941E 18	3.452E 14	3.760E 18	3.227E 22
12000	1.442E 19	5.677E 16	4.977E 23	8.062E 20	5.715E 22	4.725E 18	2.333E 14	4.436E 18	5.716E 22
13000	6.513E 18	7.732E 16	3.868E 23	1.740E 21	8.903E 22	4.791E 18	1.371E 14	4.452E 18	8.903E 22
14000	2.616E 18	8.172E 16	2.777E 23	3.003E 21	1.232E 23	4.055E 18	5.623E 13	3.747E 18	1.232E 23
15000	9.111E 17	5.681E 16	1.827E 23	3.706E 21	1.533E 23	2.858E 18	2.566E 13	2.640E 18	1.533E 23
16000	2.770E 17	3.266E 16	1.109E 23	4.090E 21	1.739E 23	1.727E 18	8.084E 12	1.587E 18	1.739E 23
18000	2.088E 16	7.889E 15	3.581E 22	3.925E 21	1.859E 23	4.695E 17	5.660E 11	4.317E 17	1.859E 23
20000	1.709E 15	1.762E 15	1.172E 22	3.331E 21	1.775E 23	1.191E 17	3.950E 10	1.098E 17	1.775E 23
22000	1.827E 14	4.423E 14	4.292E 21	2.751E 21	1.645E 23	3.356E 16	3.520E 09	3.114E 16	1.645E 23
24000	2.571E 13	1.293E 14	1.777E 21	2.299E 21	1.518E 23	1.091E 16	4.091E 08	1.014E 16	1.518E 23
26000	4.585E 12	4.328E 13	8.183E 20	1.939E 21	1.405E 23	4.008E 15	5.961E 07	3.740E 15	1.405E 23
28000	9.950E 11	1.626E 13	4.119E 20	1.661E 21	1.306E 23	1.538E 15	1.041E 07	1.535E 15	1.306E 23
30000	2.539E 11	6.737E 12	2.232E 20	1.435E 21	1.220E 23	7.315E 14	2.173E 06	6.883E 14	1.220E 23
32000	7.423E 10	2.846E 12	1.287E 20	1.225E 21	1.144E 23	3.523E 14	5.275E 05	3.328E 14	1.144E 23
34000	2.432E 10	1.293E 12	7.810E 19	1.022E 21	1.077E 23	1.509E 14	1.454E 05	1.715E 14	1.077E 23
36000	8.774E 09	6.246E 11	4.954E 19	8.603E 20	1.018E 23	9.303E 13	4.460E 04	9.325E 13	1.018E 23
38000	3.438E 09	3.179E 11	3.262E 19	7.308E 20	9.642E 22	5.557E 13	1.501E 04	5.312E 13	9.642E 22
40000	1.447E 09	1.694E 11	2.219E 19	6.257E 20	9.162E 22	3.292E 13	5.470E 03	3.151E 13	9.162E 22

[a] See fig. 2(a).

[b] With coulomb interactions between free charged particles for $T > 2000$ K.

[c] 2.447E 25 means 2.447×10^{25}, etc.

TABLE V. - Continued. NUMBER DENSITIES OF SPECIES IN HYDROGEN PLASMA[b]

(b) Pressure, 1.01325×10^{6} N/m^2 (10 atm)

Temperature, T, K	$H_2^\ddagger$	H_2^*	$H^\ddagger$	H^*	e^-	H^-	H_3^+	H_2^+	H^+
	Number density, $\hat{N}_i$, m^{-3}								
300	2.447E 26	0.	3.259E-10	0.	0.	0.	0.	0.	0.
400	1.835E 26	0.	7.744E-01	0.	0.	0.	0.	0.	0.
500	1.468E 26	0.	3.228E 05	0.	0.	0.	0.	0.	0.
600	1.223E 26	0.	1.786E 09	0.	0.	0.	0.	0.	0.
700	1.049E 26	0.	8.367E 11	0.	0.	0.	0.	0.	0.
800	9.175E 25	0.	8.385E 13	0.	0.	0.	0.	0.	0.
900	8.155E 25	0.	3.007E 15	0.	0.	0.	0.	0.	0.
1000	7.340E 25	0.	5.252E 16	0.	0.	0.	0.	0.	0.
1100	6.672E 25	0.	5.438E 17	0.	0.	0.	0.	0.	0.
1200	6.116E 25	0.	3.804E 18	0.	0.	0.	0.	0.	0.
1300	5.646E 25	0.	1.968E 19	0.	0.	0.	0.	0.	0.
1400	5.243E 25	0.	8.036E 19	0.	3.859E 04	3.559E 00	3.860E 04	0.	0.
1500	4.893E 25	0.	2.714E 20	0.	8.635E 05	1.523E 02	8.637E 05	0.	0.
1600	4.587E 25	0.	7.859E 20	0.	1.311E 07	4.475E 03	1.311E 07	0.	0.
1800	4.077E 25	9.176E-06	4.601E 21	5.117E-07	1.222E 09	1.099E 05	1.223E 09	0.	0.
2000	3.668E 25	1.359E-02	1.880E 22	1.500E-03	4.610E 10	8.803E 07	4.619E 10	0.	0.
2200	3.330E 25	4.944E 00	5.915E 22	1.024E 00	9.000E 11	3.121E 09	9.031E 11	4.468E 05	1.154E 06
2400	3.043E 25	6.755E 02	1.529E 23	2.342E 02	1.072E 13	6.005E 10	1.078E 13	3.551E 07	1.126E 08
2600	2.789E 25	4.332E 04	3.393E 23	2.309E 04	8.704E 13	7.207E 11	8.775E 13	1.445E 09	5.453E 09
2800	2.555E 25	1.527E 06	6.669E 23	1.173E 06	5.223E 14	5.948E 12	5.280E 14	3.469E 10	1.524E 11
3000	2.328E 25	3.316E 07	1.187E 24	3.497E 07	2.451E 15	3.619E 13	2.484E 15	5.451E 11	2.746E 12
3200	2.099E 25	4.827E 08	1.942E 24	6.744E 08	9.380E 15	1.708E 14	9.510E 15	6.055E 12	3.463E 13
3400	1.863E 25	5.014E 09	2.953E 24	9.051E 09	3.023E 16	6.484E 14	3.051E 16	5.034E 13	3.256E 14
3600	1.618E 25	3.896E 10	4.209E 24	8.944E 10	8.422E 15	2.041E 15	8.354E 16	3.267E 14	2.392E 15
3800	1.366E 25	2.349E 11	5.652E 24	6.799E 11	2.077E 17	5.469E 15	1.973E 17	1.703E 15	1.419E 16
4000	1.117E 25	1.131E 12	7.182E 24	4.118E 12	4.654E 17	1.282E 16	4.017E 17	7.238E 15	6.933E 16
4300	7.711E 24	8.252E 12	9.358E 24	4.265E 13	1.398E 18	3.851E 16	8.674E 17	4.353E 16	5.258E 17
4600	4.921E 24	4.124E 13	1.103E 25	3.064E 14	3.992E 18	1.023E 17	1.293E 18	1.678E 17	2.634E 18
4900	2.958E 24	1.520E 14	1.202E 25	1.638E 15	1.099E 19	2.478E 17	1.425E 18	4.493E 17	9.367E 18
5200	1.727E 24	4.445E 14	1.239E 25	6.936E 15	2.817E 19	5.387E 17	1.315E 18	9.463E 17	2.644E 19
5600	8.453E 23	1.441E 15	1.226E 25	3.607E 16	8.587E 19	1.286E 18	1.050E 18	2.051E 18	8.406E 19
6000	4.313E 23	3.832E 15	1.180E 25	1.481E 17	2.260E 20	2.641E 18	8.091E 17	3.823E 18	2.240E 20
6500	2.015E 23	1.077E 16	1.109E 25	6.759E 17	6.396E 20	5.555E 18	5.914E 17	7.275E 18	6.373E 20
7000	1.029E 23	2.604E 16	1.038E 25	2.504E 18	1.551E 21	1.029E 19	4.483E 17	1.246E 19	1.558E 21
7500	5.689E 22	5.629E 16	9.722E 24	7.882E 18	3.384E 21	1.730E 19	3.536E 17	1.973E 19	3.381E 21
8000	3.360E 22	1.114E 17	9.127E 24	2.176E 19	6.668E 21	2.697E 19	2.889E 17	2.935E 19	6.665E 21
9000	1.372E 22	3.545E 17	8.100E 24	1.223E 20	2.072E 22	5.503E 19	2.095E 17	5.610E 19	2.071E 22
10000	6.521E 21	9.050E 17	7.231E 24	5.013E 20	5.141E 22	9.423E 19	1.635E 17	9.223E 19	5.141E 22
11000	3.424E 21	1.932E 18	6.455E 24	1.613E 21	1.080E 23	1.411E 20	1.323E 17	1.347E 20	1.080E 23
12000	1.904E 21	3.528E 18	5.719E 24	4.268E 21	1.991E 23	1.391E 20	1.073E 17	1.775E 20	1.991E 23
13000	1.084E 21	5.575E 18	4.989E 24	9.589E 21	3.301E 23	2.291E 20	8.455E 16	2.129E 20	3.301E 23
14000	6.119E 20	7.655E 18	4.247E 24	1.868E 22	5.000E 23	2.517E 20	6.284E 16	2.325E 20	5.001E 23
15000	3.343E 20	8.744E 18	3.500E 24	3.009E 22	6.994E 23	2.506E 20	4.296E 16	2.307E 20	6.994E 23
16000	1.735E 20	7.789E 18	2.775E 24	3.955E 22	9.106E 23	2.263E 20	2.652E 16	2.080E 20	9.106E 23
18000	3.834E 19	4.495E 18	1.534E 24	5.355E 22	1.279E 24	1.384E 20	7.148E 15	1.272E 20	1.279E 24
20000	6.731E 18	1.812E 18	7.352E 23	5.664E 22	1.475E 24	5.214E 19	1.293E 15	5.728E 19	1.475E 24
22000	1.090E 18	6.185E 17	3.314E 23	5.178E 22	1.509E 24	2.384E 19	1.925E 14	2.207E 19	1.509E 24
24000	1.882E 17	2.060E 17	1.520E 23	4.486E 22	1.458E 24	8.962E 18	2.875E 13	8.328E 18	1.458E 24
26000	3.722E 16	7.284E 16	7.372E 22	3.783E 22	1.378E 24	3.541E 18	4.745E 12	3.305E 18	1.378E 24
28000	8.541E 15	2.810E 16	3.816E 22	3.241E 22	1.293E 24	1.502E 18	8.846E 11	1.408E 18	1.293E 24
30000	2.254E 15	1.177E 16	2.103E 22	2.782E 22	1.214E 24	6.857E 17	1.919E 11	6.452E 17	1.214E 24
32000	6.728E 14	5.269E 15	1.225E 22	2.414E 22	1.141E 24	3.345E 17	4.768E 10	3.160E 17	1.141E 24
34000	2.236E 14	2.547E 15	7.488E 21	2.102E 22	1.075E 24	1.731E 17	1.334E 10	1.641E 17	1.075E 24
36000	8.146E 13	1.296E 15	4.773E 21	1.863E 22	1.016E 24	9.433E 16	4.136E 09	8.973E 16	1.016E 24
38000	3.217E 13	6.968E 14	3.155E 21	1.657E 22	9.631E 23	5.379E 16	1.403E 09	5.133E 16	9.631E 23
40000	1.362E 13	3.877E 14	2.153E 21	1.483E 22	9.152E 23	3.191E 16	5.145E 08	3.054E 16	9.152E 23

[b] With coulomb interactions between free charged particles for T > 2000 K.

TABLE V. - Continued. NUMBER DENSITIES OF SPECIES IN HYDROGEN PLASMA[b]

(c) Pressure, 1.01325×10^7 N/m^2 (100 atm)

Temperature, T, K	$H_2^\ddagger$	H_2^*	$H^\ddagger$	H^*	e^-	H^-	H_3^+	H_2^+	H^+
	Number density, $\hat{N}_i$, m^{-3}								
400	1.835E 27	0.	2.449E 00	0.	0.	0.	0.	0.	0.
500	1.468E 27	0.	1.021E 06	0.	0.	0.	0.	0.	0.
600	1.223E 27	0.	5.647E 09	0.	0.	0.	0.	0.	0.
700	1.049E 27	0.	2.646E 12	0.	0.	0.	0.	0.	0.
800	9.175E 26	0.	2.652E 14	0.	0.	0.	0.	0.	0.
900	8.155E 26	0.	9.508E 15	0.	0.	0.	0.	0.	0.
1000	7.340E 26	0.	1.661E 17	0.	0.	0.	0.	0.	0.
1100	6.672E 26	0.	1.720E 18	0.	0.	0.	0.	0.	0.
1200	6.116E 26	0.	1.203E 19	0.	0.	0.	0.	0.	0.
1300	5.646E 26	0.	6.225E 19	0.	0.	0.	0.	0.	0.
1400	5.243E 26	0.	2.541E 20	0.	2.170E 05	5.505E 01	2.171E 05	0.	0.
1500	4.893E 26	0.	8.583E 20	0.	4.855E 06	2.895E 03	4.858E 06	0.	0.
1600	4.587E 26	0.	2.485E 21	0.	7.369E 07	7.955E 04	7.377E 07	0.	0.
1800	4.077E 26	9.176E-05	1.455E 22	1.618E-06	6.856E 09	1.953E 07	6.886E 09	0.	0.
2000	3.669E 26	1.359E-01	5.947E 22	4.744E-03	2.588E 11	1.563E 09	2.603E 11	0.	0.
2200	3.334E 26	4.950E 01	1.872E 23	3.240E 00	5.047E 12	5.537E 10	5.102E 12	7.978E 05	6.511E 05
2400	3.053E 26	6.778E 03	4.843E 23	7.420E 02	6.005E 13	1.066E 12	6.112E 13	6.359E 07	6.363E 07
2600	2.812E 26	4.368E 05	1.077E 24	7.332E 04	4.882E 14	1.284E 13	5.010E 14	2.598E 09	3.088E 09
2800	2.600E 26	1.554E 07	2.128E 24	3.742E 05	2.940E 15	1.068E 14	3.046E 15	6.273E 10	8.640E 10
3000	2.408E 26	3.430E 08	3.817E 24	1.125E 08	1.391E 16	6.607E 14	1.457E 16	9.939E 11	1.557E 12
3200	2.230E 26	5.127E 09	6.329E 24	2.197E 09	5.402E 16	3.205E 15	5.719E 16	1.117E 13	1.960E 13
3400	2.060E 26	5.543E 10	9.821E 24	3.008E 10	1.781E 17	1.270E 16	1.905E 17	9.454E 13	1.839E 14
3600	1.895E 26	4.561E 11	1.440E 25	3.057E 11	5.114E 17	4.242E 16	5.518E 17	6.305E 14	1.349E 15
3800	1.730E 26	2.973E 12	2.011E 25	2.415E 12	1.305E 18	1.223E 17	1.416E 18	3.435E 15	8.045E 15
4000	1.566E 26	1.584E 13	2.690E 25	1.537E 13	3.011E 18	3.106E 17	3.266E 18	1.571E 16	4.020E 16
4300	1.320E 26	1.409E 14	3.871E 25	1.754E 14	8.997E 13	1.025E 18	9.558E 18	1.161E 17	3.389E 17
4600	1.079E 26	8.998E 14	5.167E 25	1.421E 15	2.306E 19	2.768E 18	2.305E 19	6.390E 17	2.142E 18
4900	8.525E 25	4.345E 15	6.453E 25	8.661E 15	5.286E 19	6.397E 18	4.605E 19	2.705E 18	1.050E 19
5200	6.509E 25	1.654E 16	7.606E 25	4.163E 16	1.128E 20	1.325E 19	7.639E 19	8.952E 18	4.075E 19
5600	4.330E 25	7.218E 16	8.776E 25	2.490E 17	2.920E 20	3.131E 19	1.141E 20	3.112E 19	1.782E 20
6000	2.772E 25	2.375E 17	9.461E 25	1.125E 18	7.150E 20	6.709E 19	1.328E 20	7.828E 19	5.720E 20
6500	1.554E 25	7.828E 17	9.737E 25	5.470E 18	1.988E 21	1.516E 20	1.306E 20	1.830E 20	1.826E 21
7000	8.812E 24	2.042E 18	9.603E 25	2.064E 19	4.872E 21	2.971E 20	1.159E 20	3.482E 20	4.705E 21
7500	5.169E 24	4.526E 18	9.267E 25	6.439E 19	1.056E 22	5.193E 20	9.969E 19	5.837E 20	1.049E 22
8000	3.162E 24	8.913E 18	8.854E 25	1.735E 20	2.117E 22	8.306E 20	8.573E 19	8.978E 20	2.102E 22
9000	1.341E 24	2.692E 19	8.007E 25	9.072E 20	5.574E 22	1.752E 21	6.585E 19	1.784E 21	6.664E 22
10000	6.538E 23	6.418E 19	7.240E 25	3.439E 21	1.679E 23	3.083E 21	5.357E 19	3.017E 21	1.680E 23
11000	3.542E 23	1.290E 20	6.565E 25	1.032E 22	3.585E 23	4.768E 21	4.549E 19	4.550E 21	3.587E 23
12000	2.069E 23	2.275E 20	5.962E 25	2.586E 22	6.750E 23	6.685E 21	3.956E 19	6.279E 21	6.754E 23
13000	1.272E 23	3.602E 20	5.405E 25	5.635E 22	1.151E 24	8.656E 21	3.462E 19	8.047E 21	1.152E 24
14000	8.066E 22	5.188E 20	4.876E 25	1.094E 23	1.810E 24	1.046E 22	3.000E 19	9.667E 21	1.811E 24
15000	5.193E 22	6.856E 20	4.361E 25	1.924E 23	2.659E 24	1.188E 22	2.537E 19	1.094E 22	2.660E 24
16000	3.350E 22	7.867E 20	3.856E 25	2.896E 23	3.684E 24	1.272E 22	2.072E 19	1.169E 22	3.685E 24
18000	1.350E 22	7.307E 20	2.880E 25	4.719E 23	5.091E 24	1.237E 22	1.199E 19	1.137E 22	6.092E 24
20000	4.972E 21	5.383E 20	1.998E 25	6.460E 23	8.526E 24	9.761E 21	5.520E 18	8.999E 21	8.527E 24
22000	1.647E 21	3.242E 20	1.289E 25	7.401E 23	1.045E 25	5.422E 21	2.017E 18	5.943E 21	1.045E 25
24000	5.021E 20	1.674E 20	7.850E 24	7.515E 23	1.159E 25	3.681E 21	5.101E 17	3.421E 21	1.159E 25
26000	1.476E 20	7.916E 19	4.642E 24	7.067E 23	1.200E 25	1.943E 21	1.639E 17	1.813E 21	1.200E 25
28000	4.395E 19	3.623E 19	2.738E 24	6.346E 23	1.192E 25	9.934E 20	4.196E 16	9.310E 20	1.192E 25
30000	1.373E 19	1.665E 19	1.642E 24	5.554E 23	1.157E 25	5.101E 20	1.115E 16	4.800E 20	1.157E 25
32000	4.585E 18	8.022E 18	1.011E 24	4.798E 23	1.109E 25	2.685E 20	3.159E 15	2.536E 20	1.109E 25
34000	1.641E 18	4.032E 18	6.416E 23	4.241E 23	1.057E 25	1.459E 20	9.630E 14	1.383E 20	1.057E 25
36000	6.304E 17	2.097E 18	4.199E 23	3.754E 23	1.006E 25	8.217E 19	3.169E 14	7.816E 19	1.006E 25
38000	2.588E 17	1.142E 18	2.830E 23	3.313E 23	9.578E 24	4.798E 19	1.122E 14	4.578E 19	9.578E 24
40000	1.128E 17	6.479E 17	1.959E 23	2.960E 23	9.125E 24	2.896E 19	4.248E 13	2.771E 19	9.125E 24

[b] With coulomb interactions between free charged particles for $T > 2000$ K.

TABLE V. - Concluded. NUMBER DENSITIES OF SPECIES IN HYDROGEN PLASMA[b, d]

(d) Pressure, 1.01325×10^8 N/m^2 (1000 atm)

Temperature, T, K	$H_2^\ddagger$	H_2^*	$H^\ddagger$	H^*	e^-	H^-	H_3^+	H_2^+	H^+
	Number density, $\hat{N}_i$, m^{-3}								
1600	4.587E 27	0.	7.859E 21	0.	4.139E 08	1.413E 06	4.153E 08	0.	0.
1800	4.078E 27	9.176E-04	4.601E 22	5.118E-06	3.849E 10	3.463E 08	3.884E 10	0.	0.
2000	3.670E 27	1.360E 00	1.881E 23	1.500E-02	1.446E 12	2.762E 10	1.474E 12	0.	0.
2200	3.336E 27	4.952E 02	5.920E 23	1.025E 01	2.806E 13	9.738E 11	2.903E 13	1.435E 06	3.704E 05
2400	3.057E 27	6.786E 04	1.532E 24	2.347E 03	3.318E 14	1.863E 13	3.504E 14	1.152E 08	3.644E 07
2600	2.819E 27	4.379E 06	3.411E 24	2.321E 05	2.677E 15	2.229E 14	2.900E 15	4.749E 09	1.783E 09
2800	2.615E 27	1.562E 08	6.747E 24	1.186E 07	1.500E 15	1.844E 15	1.785E 16	1.159E 11	5.034E 10
3000	2.434E 27	3.466E 09	1.214E 25	3.572E 08	7.522E 15	1.136E 16	8.658E 16	1.858E 12	9.153E 11
3200	2.273E 27	5.224E 10	2.021E 25	7.004E 09	2.909E 17	5.510E 16	3.459E 17	2.116E 13	1.163E 13
3400	2.127E 27	5.718E 11	3.156E 25	9.641E 10	9.575E 17	2.194E 17	1.177E 18	1.817E 14	1.100E 14
3600	1.992E 27	4.790E 12	4.670E 25	9.879E 11	2.757E 18	7.414E 17	3.496E 18	1.232E 15	8.129E 14
3800	1.865E 27	3.199E 13	6.604E 25	7.891E 12	7.087E 18	2.181E 18	9.256E 18	6.838E 15	4.878E 15
4000	1.745E 27	1.761E 14	8.978E 25	5.100E 13	1.655E 19	5.698E 18	2.219E 19	3.199E 16	2.451E 16
4300	1.573E 27	1.672E 15	1.337E 26	6.001E 14	5.075E 19	1.997E 19	7.026E 19	2.468E 17	2.088E 17
4600	1.409E 27	1.168E 16	1.867E 26	5.067E 15	1.339E 20	5.807E 19	1.892E 20	1.451E 18	1.346E 18
4900	1.251E 27	6.315E 16	2.472E 26	3.258E 16	3.125E 20	1.449E 20	4.437E 20	6.805E 18	6.898E 18
5200	1.099E 27	2.755E 17	3.125E 26	1.670E 17	6.599E 20	3.184E 20	9.228E 20	2.632E 19	2.916E 19
5600	9.086E 26	1.484E 18	4.020E 26	1.103E 18	1.580E 21	7.760E 20	2.078E 21	1.238E 20	1.547E 20
6000	7.358E 26	6.125E 18	4.874E 26	5.537E 18	3.400E 21	1.541E 21	3.949E 21	4.517E 20	6.406E 20
6500	5.499E 26	2.654E 19	5.792E 26	3.054E 19	7.989E 21	3.624E 21	7.122E 21	1.677E 21	2.813E 21
7000	4.008E 26	8.745E 19	6.476E 26	1.280E 20	1.736E 22	7.142E 21	1.048E 22	4.670E 21	9.355E 21
7500	2.874E 26	2.322E 20	6.911E 26	4.313E 20	3.553E 22	1.291E 22	1.317E 22	1.034E 22	2.492E 22
8000	2.048E 26	5.205E 20	7.125E 26	1.223E 21	6.861E 22	2.166E 22	1.483E 22	1.930E 22	5.614E 22
9000	1.053E 26	1.808E 21	7.097E 26	6.643E 21	2.158E 23	5.021E 22	1.570E 22	4.799E 22	2.023E 23
10000	5.695E 25	4.507E 21	6.757E 26	2.493E 22	5.544E 23	9.496E 22	1.509E 22	9.107E 22	5.432E 23
11000	3.280E 25	9.062E 21	6.318E 26	7.254E 22	1.213E 24	1.553E 23	1.417E 22	1.473E 23	1.207E 24
12000	2.003E 25	1.570E 22	5.866E 26	1.755E 23	2.344E 24	2.284E 23	1.330E 22	2.144E 23	2.344E 24
13000	1.285E 25	2.437E 22	5.432E 26	3.692E 23	4.104E 24	3.102E 23	1.249E 22	2.888E 23	4.113E 24
14000	8.555E 24	3.469E 22	5.022E 26	6.954E 23	6.539E 24	3.951E 23	1.170E 22	3.659E 23	6.657E 24
15000	5.858E 24	4.600E 22	4.633E 26	1.198E 24	1.006E 25	4.772E 23	1.085E 22	4.404E 23	1.009E 25
16000	4.090E 24	5.715E 22	4.260E 26	1.915E 24	1.442E 25	5.501E 23	9.920E 21	5.068E 23	1.446E 25
18000	2.059E 24	6.657E 22	3.556E 26	3.416E 24	2.586E 25	6.487E 23	7.778E 21	5.974E 23	2.591E 25
20000	1.047E 24	6.373E 22	2.900E 26	4.936E 24	4.003E 25	6.651E 23	5.466E 21	6.139E 23	4.007E 25
22000	5.248E 23	5.355E 22	2.300E 26	5.140E 24	5.512E 25	6.345E 23	3.391E 21	5.598E 23	5.516E 25
24000	2.552E 23	4.078E 22	1.770E 26	7.225E 24	6.907E 25	4.945E 23	1.848E 21	4.598E 23	6.910E 25
26000	1.203E 23	2.868E 22	1.325E 26	7.916E 24	8.035E 25	3.713E 23	8.946E 20	3.466E 23	8.037E 25
28000	5.535E 22	1.871E 22	9.715E 25	8.132E 24	8.827E 25	2.610E 23	3.913E 20	2.447E 23	8.829E 25
30000	2.512E 22	1.156E 22	7.020E 25	7.963E 24	9.291E 25	1.753E 23	1.638E 20	1.649E 23	9.292E 25
32000	1.138E 22	6.899E 21	5.037E 25	7.530E 24	9.483E 25	1.144E 23	6.705E 19	1.080E 23	9.483E 25
34000	5.205E 21	4.062E 21	3.613E 25	6.944E 24	9.472E 25	7.359E 22	2.736E 19	6.977E 22	9.472E 25
36000	2.424E 21	2.400E 21	2.604E 25	6.333E 24	9.323E 25	4.721E 22	1.129E 19	4.491E 22	9.323E 25
38000	1.153E 21	1.434E 21	1.889E 25	5.912E 24	9.081E 25	3.036E 22	4.741E 18	2.898E 22	9.081E 25
40000	5.648E 20	8.677E 20	1.386E 25	5.467E 24	8.794E 25	1.975E 22	2.050E 18	1.890E 22	8.795E 25

[b] With coulomb interactions between free charged particles for T > 2000 K.

[d] See fig. 2(b).

TABLE VI. - INPUT FORM WITH DATA FOR SAMPLE PROBLEMS FOR COMPUTER PROGRAM FOR COMPONENTS OF HYDROGEN PLASMA

[Top row of numbers are card column numbers.]

a

1 10	11 25	26 30
DH	PD	IPR
1.	1.01325E+8	0

1 10	11 15
T	IFLAG
30000.	1

b

1 10	11 25	26 30
DH	PD	IPR
1.	1.01325E+8	1

1 10	11 15
T	IFLAG
300.	0
1500.	0
10000.	0
20000.	0
30000.	0
40000.	0

[a] Case 1.

[b] Cases 2 to 7.

TABLE VII. - OUTPUT FOR SAMPLE PROBLEMS FOR COMPUTER PROGRAM FOR

COMPONENTS OF HYDROGEN PLASMA

```
a {DH  1.0000E 00     PD  1.0132E 08     IPR  0

  PRESSURE  1.0132E 08 N/M**2     TEMP.  3.0000E 04 K     DENSITY  2.8727E-01 KG/M**3     TOTAL NUMBER DENSITY  2.6438E 26 1/M**3
  COULOMB COMPRESSIBILITY  0.92540     RECIPROCAL DEBYE LENGTH  1.1415E 09 1/M     EQUIV. CONC./CRITICAL EQUIV. CONC.  4.6571E-01

  SPECIES NUMBER DENSITY, PARTICLES/CUBIC METER
   H  7.8165E 25     H+  9.2924E 25     E  9.2914E 25     H2  3.6576E 22     H-  1.7525E 23     H2+  1.6494E 23     H3+  1.5378E 20

  DETAILED NUMBER DENSITY FOR H2, MOLECULES/CUBIC METER
   GROUND ELECTRONIC STATE WITH VIBRATIONAL QUANTUM NUMBER OF   V=0    4.9227E 21     V=1    4.0348E 21     V=2    3.3416E 21
    V=3    2.7657E 21     V=4    2.2841E 21     V=5    1.8795E 21     V=6    1.5383E 21     V=7    1.2499E 21     V=8    1.0062E 21
    V=9    7.0289E 20     V=10   5.3901E 20     V=11   4.0382E 20     V=12   2.7185E 20     V=13   1.3668E 20     V=14   3.9788E 19
   1SNS SINGLET SIGMA STATES WITH               N=1    2.5117E 22     N=2    3.3399E 20     N=3    8.1356E 19     N=4    0.
   1SNP SINGLET SIGMA STATES WITH               N=2    3.1471E 21     N=3    4.3593E 19     N=4    0.
   1SNP SINGLET PI STATES WITH                  N=2    6.1915E 20     N=3    1.5213E 20     N=4    0.
   1SND SINGLET SIGMA STATES WITH               N=3    2.2879E 19     N=4    0.
   1SND SINGLET PI STATES WITH                  N=3    4.9196E 19     N=4    0.
   1SND SINGLET DELTA STATES WITH               N=3    1.8396E 20     N=4    0.
   1S4F SINGLET SIGMA STATE                            0.
   1S4F SINGLET PI STATE                               0.
   1S4F SINGLET DELTA STATE                            0.
   1S4F SINGLET PHI STATE                              0.
   1SNS TRIPLET SIGMA STATES WITH               N=2    1.3200E 21     N=3    3.2367E 20     N=4    0.
   1SNP TRIPLET SIGMA STATES WITH               N=3    3.4661E 20     N=4    7.3138E 17
   1SNP TRIPLET PI STATES WITH                  N=2    3.3393E 21     N=3    6.9445E 20     N=4    0.
   1SND TRIPLET SIGMA STATES WITH               N=3    1.4995E 20     N=4    0.
   1SND TRIPLET PI STATES WITH                  N=3    1.7767E 20     N=4    0.
   1SND TRIPLET DELTA STATES WITH               N=3    5.6859E 20     N=4    0.
   1S4F TRIPLET SIGMA STATE                            0.
b  1S4F TRIPLET PI STATE                               0.
   1S4F TRIPLET DELTA STATE                            0.
   1S4F TRIPLET PHI STATE                              0.
   ALL 1SN STATES WITH                          N=5    0.             N=6    0.             N=7    0.             N=8    0.
    N=9    0.             N=10   0.             N=11   0.             N=12   0.             N=13   0.             N=14   0.
    N=15   0.             N=16   0.             N=17   0.
   TOTAL IN EXCITED ELECTRONIC STATES                  1.1559E 22

  DETAILED NUMBER DENSITY FOR H, ATOMS/CUBIC METER
   STATES WITH PRINCIPAL QUANTUM NUMBER OF   N=1    7.0202E 25     N=2    5.4332E 24     N=3    2.5298E 24     N=4    0.
    N=5    0.             N=6    0.             N=7    0.             N=8    0.             N=9    0.             N=10   0.
    N=11   0.             N=12   0.             N=13   0.             N=14   0.             N=15   0.             N=16   0.
    N=17   0.
   TOTAL IN EXCITED ELECTRONIC STATES                  7.9631E 24

  DETAILED NUMBER DENSITY FOR H2+, IONS/CUBIC METER
   GROUND ELECTRONIC STATE WITH VIBRATIONAL QUANTUM NUMBER OF   V=0    2.3509E 22     V=1    2.0679E 22     V=2    1.8133E 22
    V=3    1.6150E 22     V=4    1.4071E 22     V=5    1.2195E 22     V=6    1.0503E 22     V=7    9.7655E 21     V=8    8.3513E 21
    V=9    7.0784E 21     V=10   5.9367E 21     V=11   4.9174E 21     V=12   4.0127E 21     V=13   3.2155E 21     V=14   2.5196E 21
    V=15   1.9189E 21     V=16   1.0869E 21     V=17   6.3669E 20     V=18   2.1027E 20     V=19   4.6708E 19

  MISCELLANEOUS QUANTITIES
   DELI         1.3258E 06      DELIN        1.3258E 06      RD           1.1167E-09      RON          1.1167E-09
   CUT1         4.5937E 00      CUT2         2.8764E 00      Q(1)         2.2259E 00      Q4P          1.8398E 03
   Q6P          6.3329E 03      Q7P          8.2173E 06      ERETA       -7.9684E-11      C            8.0847E-14
   ERS         -3.9636E-09      DELLV       -5.6884E-08      DELLGM(1) 2.5241E-07        DELLGM(2)-2.1141E-07
   DELLGM(3)-2.1141E-07         DELLGM(4) 2.5176E-07         DELLGM(5)-2.1206E-07        DELLGM(6)-2.1206E-07
   DELLGM(7)-2.1271E-07         ETAD         3.0000E 00      I1           4               I2           6

c {DH  1.0000E 00     PD  1.0132E 08     IPR  1

    300     2.447E 28  0.         3.259E-09  0.         0.         0.         0.         0.         0.         2.447E 28  3.259E-09
   1500     4.893E 27  0.         2.714E 21  0.         2.728E 07  5.145E 04  2.734E 07  0.         0.         4.893E 27  2.714E 21
  10000     5.695E 25  4.507E 21  6.757E 26  2.493E 22  5.544E 23  9.496E 22  1.509E 22  9.107E 22  5.432E 23  5.695E 25  5.758E 25
d 20000     1.047E 24  6.373E 22  2.900E 26  4.936E 24  4.003E 25  5.651E 23  5.456E 21  6.139E 23  4.007E 25  1.111E 24  2.950E 25
  30000     2.512E 22  1.156E 22  7.020E 25  7.963E 24  9.291E 25  1.753E 23  1.638E 20  1.649E 23  9.292E 25  3.668E 22  7.815E 25

  40000     5.648E 20  8.677E 20  1.386E 25  5.467E 24  8.794E 25  1.975E 22  2.050E 18  1.890E 22  8.795E 25  1.432E 21  1.933E 25
```

[a] First page of case 1.

[b] Second page of case 1.

[c] First page of cases 2 to 7.

[d] Second page of cases 2 to 7.

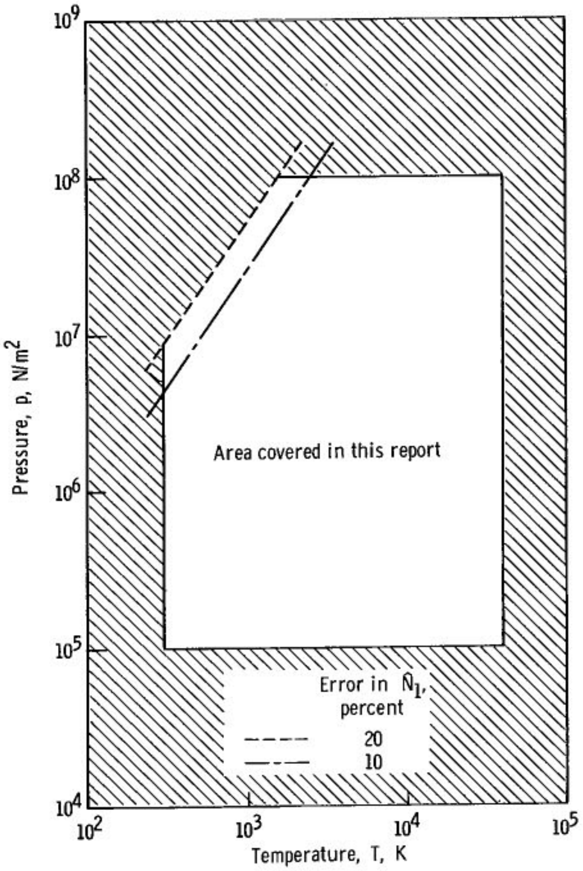
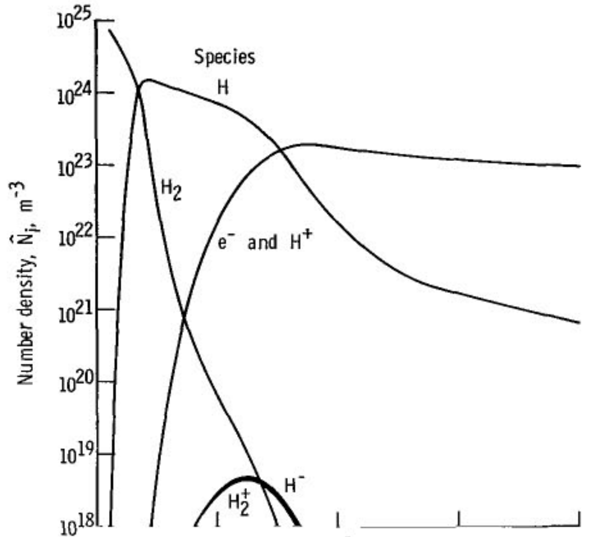
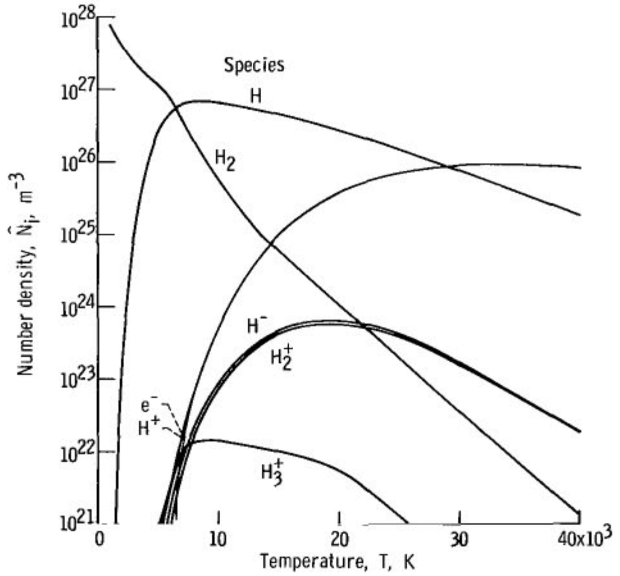


Figure 1. - Pressures and temperatures covered in this report. Error in $\hat{N}_1$ in upper left-hand corner was excessive because of neglect of intermolecular forces between neutral species.



(a) At pressure of 1.01325x10^5 newtons per square meter (1 atm).



(b) At pressure of 1.01325x10^8 newtons per square meter (1000 atm).

Figure 2. - Number densities of components of hydrogen plasma with coulomb interactions between free charged particles for T > 2000 K.

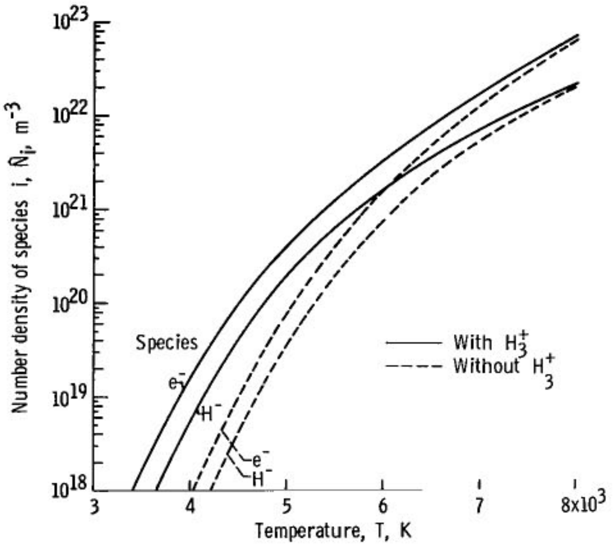


Figure 3. - Calculated number densities of e^- and H^- in hydrogen plasma at pressure of 1.01325×10^8 newtons per square meter (1000 atm) with and without H_3^+. Coulomb interactions between free charged particles were included.

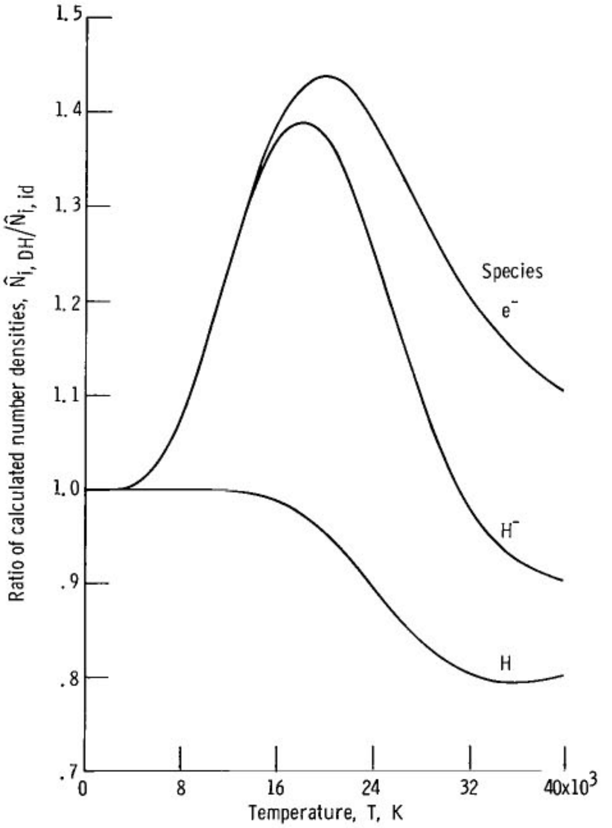


Figure 4. - Ratio of calculated number densities of H, e^-, and H^- with and without coulomb interactions between free charged particles. Pressure of 1.01325×10^8 newtons per square meter (1000 atm).

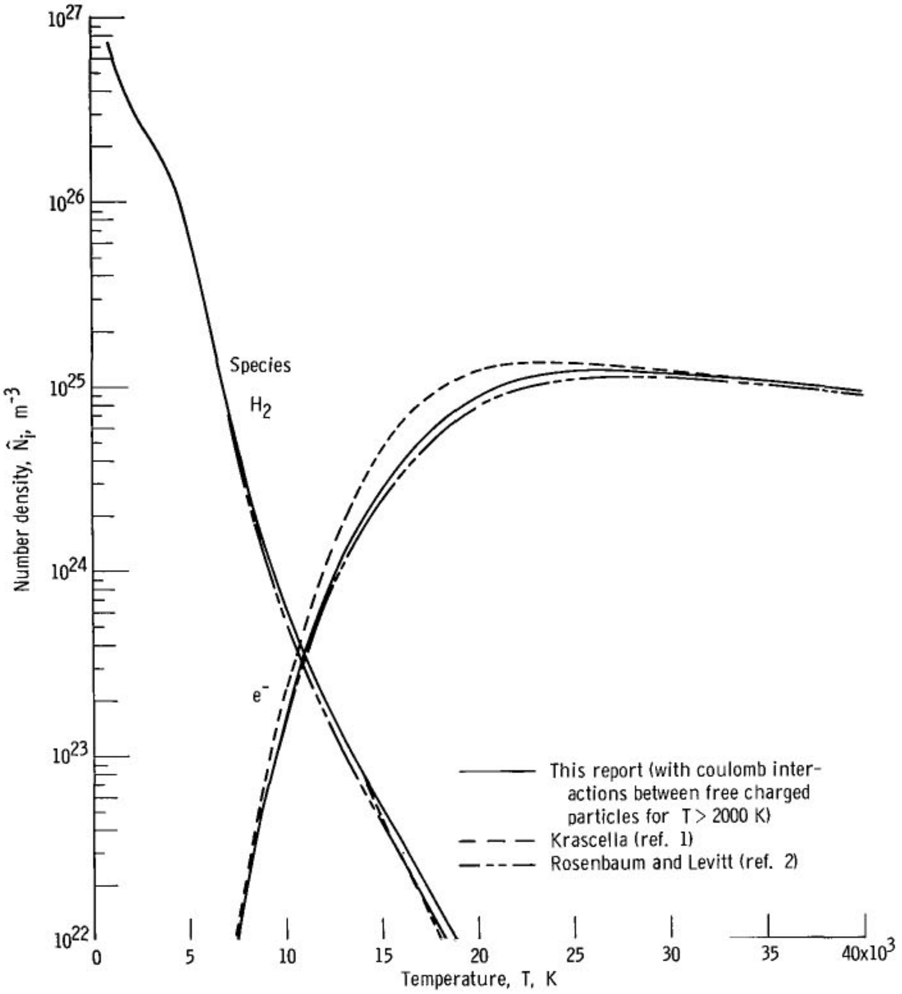


Figure 5. - Number densities of H_2 molecules and free electrons in hydrogen plasma calculated by different investigators at pressure of 1.01325×10^7 newtons per square meter (100 atm).

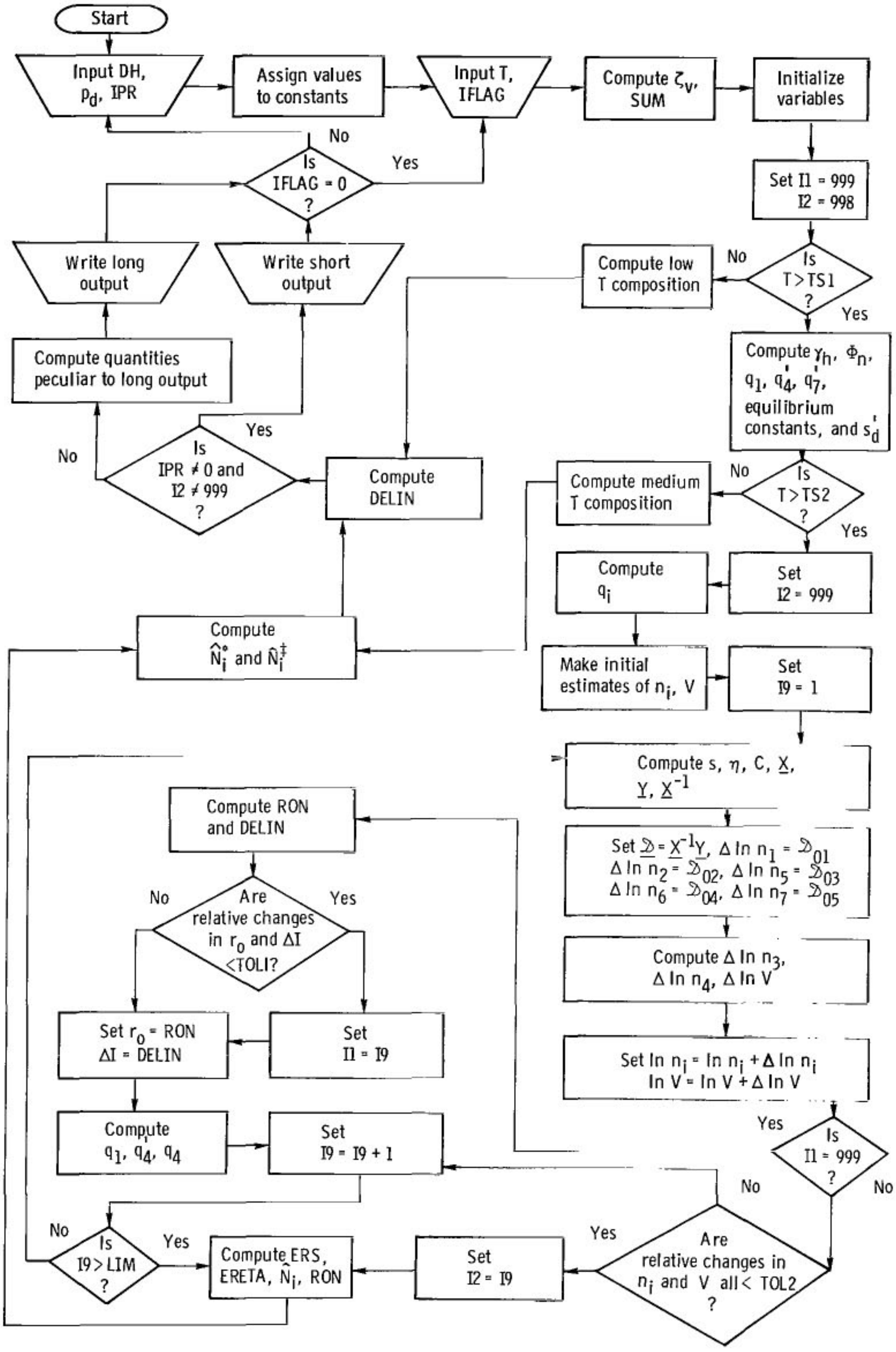


Figure 6. - Simplified flow diagram for computer program for components of hydrogen plasma.

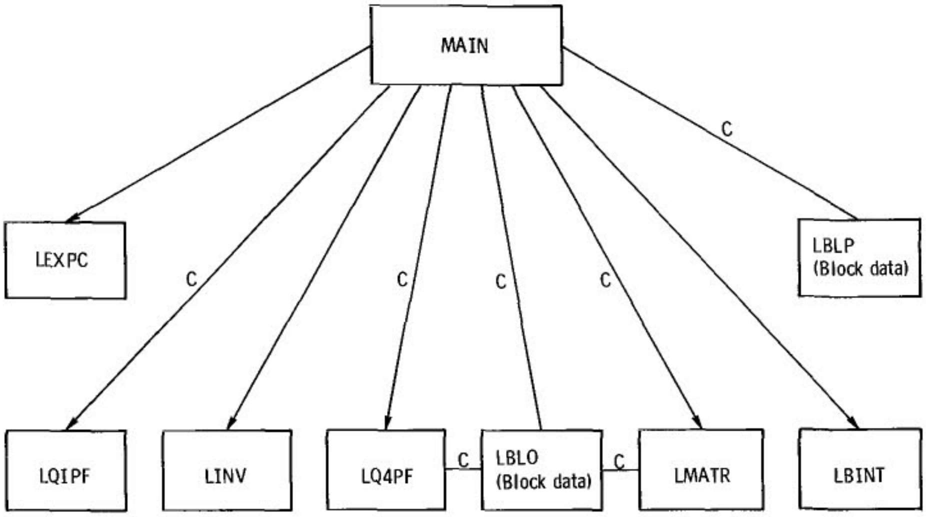


Figure 7. - Block diagram of program and subprograms for components of hydrogen plasma. Direction of call is indicated by arrowhead. Common storage is indicated by C.

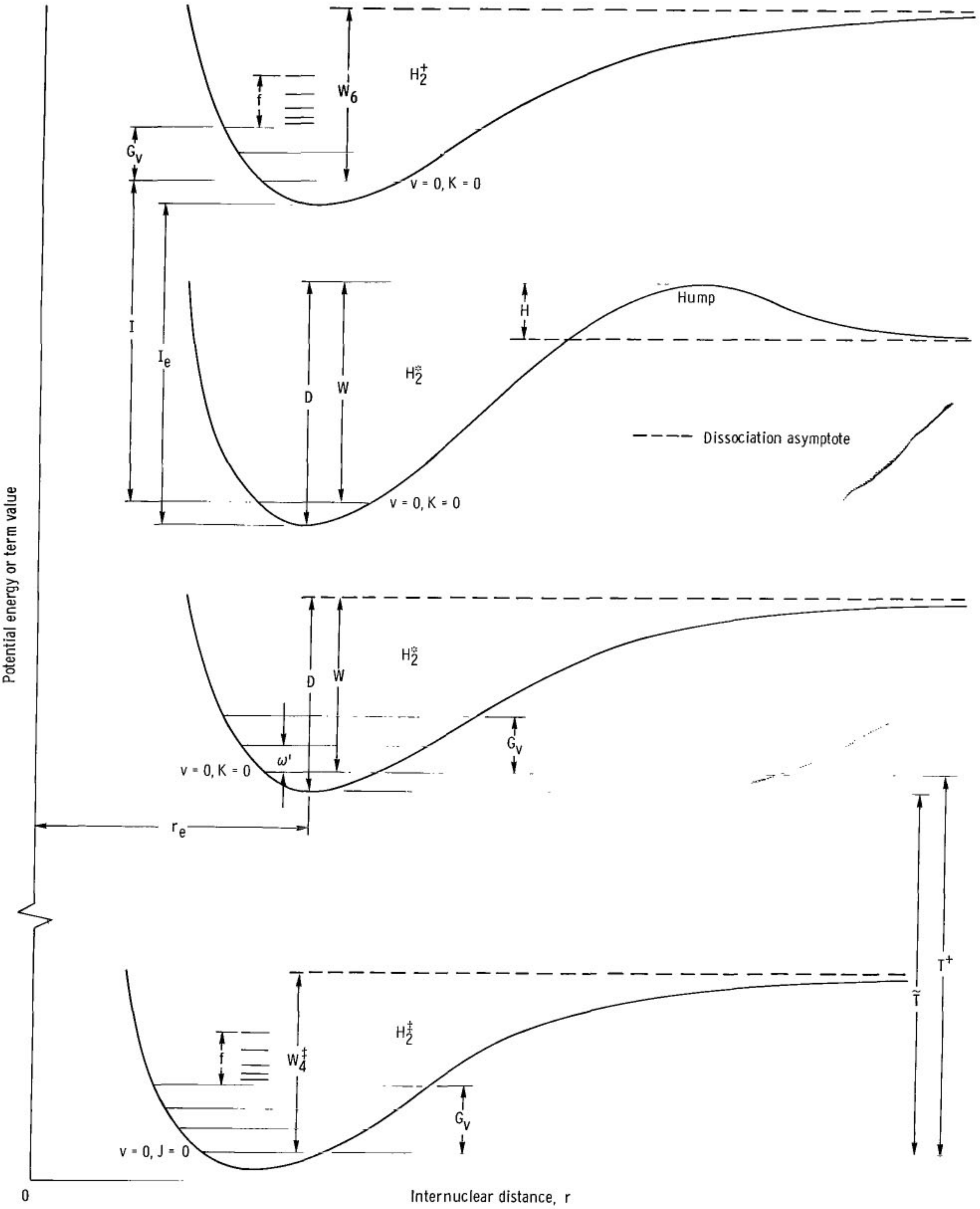


Figure 8. - Potential energies and term values of ground state of H_2^+, two excited electronic states of H_2 (labeled H_2^*), and ground electronic state of H_2 (labeled $H_2^\ddagger$) (not to scale).

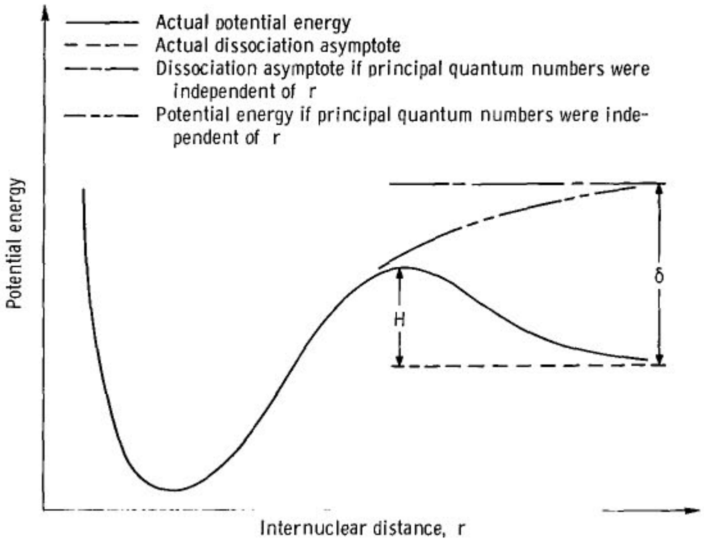


Figure 9. - Quantities in approximation for hump height for excited electronic state H_2^* with promoted molecular orbital. (Not to scale.)

NASA-Langley, 1969 — 25 E-4346