NASA TECHNICAL NOTE

NASA TN D-3538

c.1

LOAN COPY
AFWL
KIRTLAND EX
TECH LIBRARY KAFB, NM
0130287

NASA TN D-3538

CALCULATION OF THERMODYNAMIC PROPERTIES OF ARBITRARY GAS MIXTURES WITH MODIFIED VIBRATIONAL-ROTATIONAL CORRECTIONS

by Dennis O. Allison

Langley Research Center
Langley Station, Hampton, Va.

28 SEP
Technical Library
AF Weapons
Laboratory

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION • WASHINGTON, D. C. • AUGUST 1966

TECH LIBRARY KAFB, NM

0130287

NASA TN D-3538

CALCULATION OF THERMODYNAMIC PROPERTIES OF ARBITRARY GAS MIXTURES WITH MODIFIED VIBRATIONAL-ROTATIONAL CORRECTIONS

By Dennis O. Allison

Langley Research Center
Langley Station, Hampton, Va.

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

For sale by the Clearinghouse for Federal Scientific and Technical Information
Springfield, Virginia 22151 – Price $2.00

CALCULATION OF THERMODYNAMIC PROPERTIES OF ARBITRARY GAS MIXTURES WITH MODIFIED VIBRATIONAL-ROTATIONAL CORRECTIONS

By Dennis O. Allison
Langley Research Center

SUMMARY

Equilibrium thermodynamic properties are computed for mixtures of ideal gases including ionization and dissociation. Vibrational-rotational corrections for diatomic species are treated by using a modified method and results are compared with those obtained by a direct-summation method. The modified method takes an order of magnitude less computer time and retains the accuracy of the direct-summation method. Thermodynamic properties are also computed with the rotating harmonic-oscillator model for the diatomic species for comparison purposes. Calculations are made for temperatures up to 15 000° K and pressures up to 100 atmospheres. It is shown that the present diatomic corrections account for most of the difference between the rotating harmonic-oscillator and the virial methodology results for the temperatures and pressures considered. Results are given for three gas mixtures: 100 percent CO_2, a "Mars" atmosphere, and air.

INTRODUCTION

Equilibrium high-temperature thermodynamic properties of arbitrary gas mixtures are required for the study of flight in planetary atmospheres such as the atmospheres of Earth, Mars, and Venus. Many calculations have been carried out for air (refs. 1 to 10) and a few for model atmospheres of Mars and Venus (refs. 11 to 13). Most of these calculations include the effects of approximate vibrational-rotational corrections for the diatomic species. These corrections are usually made by using the method of Mayer and Mayer (ref. 14).

Diatomic corrections in this paper have been treated by a direct-summation method as well as by a modified method. The derivation of the method of Mayer and Mayer (ref. 14) contains an intermediate step which closely resembles the present modified method for diatomic corrections. Also references 15, 16, and 17 give properties of N_2 and O_2 obtained by using essentially the modified method. In the present paper, results based on the direct-summation and modified methods as well as on the rotating harmonic-oscillator method (using the harmonic-oscillator energy plus the rigid-rotor energy) are compared with one another. The direct-summation method is taken to be the most accurate of the three methods for the temperature and pressure ranges considered. Both the direct-summation and the modified method employ an approximate cutoff criterion to terminate the summations. This approximation is shown to have a negligible effect on the accuracy of mixture properties under the conditions of the present calculations.

The assumption of a mixture of ideal gases is made and dissociation and ionization are included. Twenty-six species are considered: N_2, O_2, NO, CO, CN, CO_2, N, O, C, Ar, N_2^+, O_2^+, O_2^-, NO^+, CO^+, N^+, N^{++}, O^+, O^{++}, O^-, C^+, C^{++}, C^-, Ar^+, Ar^{++}, e^-. Calculations are made for temperatures up to 15 000° K and pressures ranging from 10^{-4} to 10^2 atmospheres. The White method (sometimes called the RAND method, ref. 18) is used to determine the equilibrium composition of the mixture at a given temperature and pressure by minimizing the Gibbs free energy. Molecular-weight ratio (sometimes called compressibility factor), nondimensional enthalpy and entropy, mass density, and electron number density are computed for the mixture. In the previously described calculations, the Gibbs free energy and enthalpy for individual species are computed from the partition function of statistical mechanics.

The computer program is set up in such a way that the composition of the gas is specified by input quantities and thermodynamic properties can be computed for arbitrary gas mixtures. Calculations were made for air, CO_2, and a "Mars" atmosphere. Carbon dioxide is of interest since model atmospheres for Venus and Mars have been proposed with a 100-percent CO_2 composition. Results from the direct-summation, modified, and rotating harmonic-oscillator methods are compared for the three mixtures as well as for the species N_2 and O_2.

A more sophisticated gas model than the present one has been used by others in recent air calculations (refs. 7 to 10); for example, Browne (ref. 8) used the virial methodology for diatomic species at high temperatures. The present results for air are compared with those of Browne as an accuracy check. In addition, comparisons are made with the results of Gilmore (refs. 1 and 5) who used the assumption of a mixture of ideal gases.

SYMBOLS

a_{ik}	number of atoms of component k per particle of species i
b_k	number of moles of component k per mass of mixture, moles/g
c	speed of light, 2.99793×10^{10}, cm/sec

D_o	dissociation energy, cm^{-1}
e_i	internal energy per mole of species i, ergs/mole
f_i	Gibbs free energy per mole of species i, ergs/mole
F	Gibbs free energy of mixture (per mole of undissociated mixture), ergs/mole
g	degeneracy of an energy level
h	Planck's constant, 6.62517×10^{-27}, erg-sec
h_{oi}	standard heat of formation at $T = 0^o$ K per mole of species i, ergs/mole
h_i	enthalpy per mole of species i, ergs/mole
H	enthalpy of mixture (per mole of undissociated mixture), ergs/mole
j	rotational quantum number
k	Boltzmann constant, 1.38044×10^{-16}, ergs/deg
m	total number of components in mixture
M	molecular weight, g/mole
M_u	molecular weight of undissociated mixture, g/mole
n	total number of species considered
N_e	electron number density, cm^{-3}
N_o	Avogadro's number, 6.02322×10^{23}, $mole^{-1}$
p	pressure, $dynes/cm^2$
p_o	reference pressure (taken to be 1 atmosphere in this paper), 1.01325×10^6, $dynes/cm^2$
Q	partition function
R	universal gas constant, N_ok, ergs/mole-deg
s_i	entropy per mole of species i, ergs/mole-deg
S	entropy of mixture (per mole of undissociated mixture), ergs/mole-deg
T	absolute temperature, ^oK

T_o	reference temperature, 273.15, ^oK
v	vibrational quantum number
V	volume, cm^3
y_i	number of moles of species i per mass of mixture, moles/g
$\bar{y}$	total number of moles per mass of mixture, moles/g
Z	molecular weight ratio
Δ	property difference
ϵ	energy, ergs
$(\nu_e)_l$	difference in energy of minima of potential curves of ground state and l th electronic state, cm^{-1}
ν_l	l th electronic energy level, cm^{-1}
ρ	mass density, g/cm^3
ρ_o	reference mass density, $\frac{p_o}{\bar{y}RT_o}$, g/cm^3
σ	symmetry number
$\omega_e, \omega_e x_e, B_e, \alpha_e, D_e$	spectroscopic constants for vibrational-rotational energies, cm^{-1}

Subscripts:

i	species index
int	internal
k	component index
l	electronic energy level index
max	maximum value
rot	rotational
s	quantum energy state
tr	translational

vib	vibrational
w	vibrational frequency index

METHOD

Model of Arbitrary Gas Mixture

Calculations are made by assuming a mixture of ideal gases for temperatures up to 15 000° K and pressures from $10^{-4}p_o$ to $10^2 p_o$. A given gas mixture is derived from atomic elements or components with electrons taken to be a component when ionization is considered. The components and chemical combinations of the components, including positive and negative ions, form the list of species. All species which can form in appreciable amounts at the temperatures and pressures of interest should be included. Five components (N, O, C, Ar, e^-) and 26 species are considered in the present work: N, O, C, Ar, N_2, O_2, NO, CO, CN, CO_2, N^+, N^{++}, O^+, O^{++}, O^-, C^+, C^{++}, C^-, Ar^+, Ar^{++}, N_2^+, O_2^+, O_2^-, NO^+, CO^+, e^-.

It is well known that translational and internal modes must be considered for each species where rotational, vibrational, and electronic states are the internal modes. The energy modes of a given species will appear in its partition function from which thermodynamic properties are computed.

All thermochemical and spectroscopic constants used in the calculations are given in tables I to III with source references.

Partition Functions

The partition function Q for any one species is defined as the following sum over all the quantum energy states of the species:

$$Q = \sum_s g_s e^{-\epsilon_s/kT} \tag{1}$$

Since the translational energies are independent of the internal energies, the partition function can be written as a product of a translational and an internal partition function

$$Q = Q_{tr} Q_{int} \tag{2}$$

The translational partition function takes the familiar form (ref. 19)

$$Q_{tr} = \left(\frac{2\pi MkT}{N_0h^2}\right)^{3/2} V = \left(\frac{2\pi MkT}{N_0h^2}\right)^{3/2} \frac{kT}{p} \tag{3}$$

The internal partition function differs for the three types of species: atomic, diatomic, and linear triatomic. For atomic species only electronic states are considered in Q_{int}; therefore,

$$Q_{int} = \sum_{l} g_l e^{-\frac{hc}{kT}\nu_l} \tag{4}$$

where the sum should be taken over all electronic energy states which are significantly occupied at the temperatures and pressures of interest. Since the reasoning of Gilmore (ref. 1) is followed, all levels for which the principal quantum number is less than or equal to 5 are included. In addition to observed levels (ref. 20), a large number of missing levels that could be approximated by extrapolating along the isoelectronic sequences (ref. 21) are included. All levels for which the energies are greater than the ionization potential were omitted and many of the high energy levels were grouped together by adding their degeneracies and assigning them an average energy. Further discussion of the electronic energy levels used can be found in appendix B of reference 22.

For diatomic species the internal partition function includes vibrational and rotational energies

$$Q_{int} = \sum_{l} \left(Q_{vib,rot}\right)_l g_l e^{-\frac{hc}{kT}\nu_l} \tag{5}$$

Electronic energy levels with $\nu_l > 90\,000 \text{ cm}^{-1}$ were not included. For each electronic energy level

$$Q_{vib,rot} = \frac{1}{\sigma} \sum_{v=0}^{v_{max}} \sum_{j=0}^{j(v)_{max}} g(v,j)e^{-\epsilon(v,j)/kT} \tag{6}$$

where v and j are the vibrational and rotational quantum numbers, respectively, and σ is the symmetry number (refs. 14 and 23). For a given v and j

$$g(v,j) = 2j + 1 \tag{7}$$

and, if the third and higher powers of v and j(j + 1) are neglected, the vibrational-rotational energy is

$$\epsilon(v,j) = hc\left[\left(\omega_e - \omega_e x_e\right)v + \left(B_e - \frac{1}{2}\alpha_e\right)j(j + 1) - \omega_e x_e v^2 - \alpha_e vj(j + 1) - D_e j^2(j + 1)^2\right] \tag{8}$$

which is useful for values of v and j that significantly contribute to thermodynamic properties. Use of this quadratic energy expression is justified in the section "Comparison With Other Results." The first two terms are the harmonic-oscillator and rigid-rotor energies, respectively, and the last three terms are first-order corrections (refs. 14 and 23). The heat of formation h_{oi} includes the constant terms which do not appear in equation (8). The spectroscopic constants satisfy the inequalities

$$\omega_e \gg \omega_e x_e > B_e \gg \alpha_e \gg D_e \tag{9}$$

Since ω_e, $\omega_e x_e$, B_e, and α_e are available in the literature, it is convenient to determine D_e in terms of these quantities. The Morse potential can be used to obtain the approximate equation for D_e (refs. 14 and 23)

$$D_e = \frac{4B_e^3}{\omega_e^2} \tag{10}$$

which is used throughout the calculations. To complete the expression for $Q_{vib,rot}$, v_{max} and $j(v)_{max}$ must be specified. The partition function $Q_{vib,rot}$ is not very sensitive to these upper limits on v and j because $\epsilon(v,j)$ appears as a negative exponent in equation (6). Therefore, approximate values of v_{max} and $j(v)_{max}$ can be used. First, the dissociation energy D_o is needed for each electronic state. The ground state D_o is generally known, but D_o for excited electronic states is not readily available and approximate values were determined as follows: Consider the energy expression (eq. (8)) for $j = 0$

$$\epsilon(v,0) = hc\left[(\omega_e - \omega_e x_e)v - \omega_e x_e v^2\right] \tag{11}$$

and notice that as v increases, $\epsilon(v,0)$ reaches a maximum and then decreases. (See fig. 1(a).) This highest energy value is taken to be the dissociation energy hcD_o; thus, D_o is given by

$$D_o = \frac{(\omega_e - \omega_e x_e)^2}{4\omega_e x_e} \tag{12}$$

for excited electronic states (ref. 23). This expression can also be obtained by using a Morse potential. Approximate values of v_{max} and $j(v)_{max}$ were obtained by allowing all v and j for which the sum of the harmonic-oscillator energy plus the rigid-rotor energy is less than the dissociation energy hcD_o; that is,

$$(\omega_e - \omega_e x_e)v + \left(B_e - \frac{\alpha_e}{2}\right)j(j + 1) < D_o \tag{13}$$

For the ground state, an experimental value of D_0 is used, and the D_0 from equation (12) is used for an excited electronic state. The upper limit v_{max} is taken to be the largest integer for which equation (13) is satisfied for $j = 0$. For all $v \leqq v_{max}$, $j(v)_{max}$ is taken to be the largest integer for which equation (13) holds. Figure 1 shows graphically how v_{max} and $j(v)_{max}$ are determined for an excited electronic state. In figure 1(a) the curved line is used to determine D_0 for excited electronic states as explained above. The straight line corresponds to the harmonic-oscillator energy and is used to determine v_{max} for the ground electronic state as well as for the excited electronic states. Thus, for excited electronic states, v_{max} happens to be only one-half the magnitude of the v at which $\epsilon(v,0)$ reaches its highest value. If v_{max} were any larger, unrealistic (negative or imaginary) values of $j(v)_{max}$ would result from equation (13). Figure 1(b) shows how the maximum value of $j(j + 1)$ and consequently of j is determined for a given v. A maximum j is determined for each v from $v = 0$ to $v = v_{max}$.

Use of this vibrational-rotational cutoff criterion is justified in the section "Comparison With Other Results." The quantity $Q_{vib,rot}$ can now be computed from equation (6). Unfortunately, $j(v)_{max}$ is about 100 whereas v_{max} is approximately 25; thus, an excessive amount of computer time is required to compute $Q_{vib,rot}$ for each electronic energy level. To eliminate this difficulty, equation (6) was approximated to eliminate the summation over j. The approximations are discussed and the derivation of the following modified expression for $Q_{vib,rot}$ is presented in the appendix:

$$Q_{vib,rot} = \frac{1}{\sigma} \sum_{v=0}^{v_{max}} e^{-\frac{hc}{kT}\left[(\omega_e - \omega_e x_e)v - \omega_e x_e v^2\right]} \left[\frac{kT}{hc\left(B_e - \frac{1}{2}\alpha_e - \alpha_e v\right)} + \frac{8B_e^3 k^2 T^2}{\omega_e^2 h^2 c^2 \left(B_e - \frac{1}{2}\alpha_e - \alpha_e v\right)^3} + \frac{1}{3}\right] \tag{14}$$

Equation (14) is a compromise between the direct-summation method (eq. (6)) and the method of Mayer and Mayer (ref. 14). It is a useful approximation in that little computer time is consumed by the summation over v and the resulting mixture properties are almost the same as those computed with equation (6). The rotating harmonic-oscillator approximation can be made by omitting the correction terms in $\epsilon(v,j)$ (eq. (8)), and letting $v_{max} = j(v)_{max} = \infty$; therefore, equation (6) becomes

$$Q_{vib,rot} = \frac{1}{\sigma} \sum_{v=0}^{\infty} e^{-\frac{hc}{kT}(\omega_e - \omega_e x_e)v} \sum_{j=0}^{\infty} (2j + 1) e^{-\frac{hc}{kT}\left(B_e - \frac{1}{2}\alpha_e\right) j(j+1)} \tag{15}$$

The summation over v has a closed form whereas the summation over j is usually approximated by an integral (ref. 19) which is equivalent to the first term of the

Euler-Maclaurin summation formula. (See appendix.) For a given electronic energy level, the result is

$$Q_{vib,rot} = \frac{1}{\sigma}\left[1 - e^{-\frac{hc}{kT}(\omega_e - \omega_e x_e)}\right]^{-1}\left[\frac{hc}{kT}\left(B_e - \frac{1}{2}\alpha_e\right)\right]^{-1} \tag{16}$$

Mixture properties computed from each of the forms of $Q_{vib,rot}$ for diatomic species (eqs. 6, 14, and 16) are compared in the section "Results and Discussion."

Linear triatomic species are assumed to have only a ground electronic state and the harmonic-oscillator rigid-rotor model is used for the vibrations and rotations. Since a linear triatomic species has four independent vibrational frequencies, the vibrational partition function will be a product of four contributions as indicated in the following equation:

$$Q_{int} = \frac{1}{\sigma}g_o\left[\frac{hc}{kT}\left(B_e - \frac{1}{2}\alpha_e\right)\right]^{-1}\prod_{w=1}^{4}\left[1 - e^{-\frac{hc}{kT}(\omega_e - \omega_e x_e)_w}\right]^{-1} \tag{17}$$

which is derived in the same way as equation (16).

Species Properties

The expressions for species properties in terms of the partition function can be found in textbooks on statistical mechanics. The internal energy per mole of species i is

$$e_i = RT^2\left(\frac{\partial \log_e Q_i}{\partial T}\right)_V + h_{oi} = \frac{RT^2}{Q_i}\left(\frac{\partial Q_i}{\partial T}\right)_V + h_{oi} \tag{18}$$

and the enthalpy per mole is simply

$$h_i = e_i + RT \tag{19}$$

Entropy per mole is arbitrary to within an additive constant and is usually taken to be (refs. 1, 8, and 19)

$$s_i = R\left(\frac{\partial T \log_e Q_i}{\partial T}\right)_V + R = R \log_e Q_i + \frac{RT}{Q_i}\left(\frac{\partial Q_i}{\partial T}\right)_V + R \tag{20}$$

The Gibbs free energy can be determined from equations (19) and (20) as

$$f_i = h_i - Ts_i = -RT \log_e Q_i + h_{oi} \tag{21}$$

The Gibbs free energy and enthalpy are needed in determining the equilibrium composition and mixture properties.

Equilibrium Composition

To determine equilibrium at a constant temperature and pressure, the Gibbs free energy of the mixture is minimized, subject to the following constraints on the components:

$$b_k = \sum_{i=1}^{n} a_{ik} y_i \qquad (k = 1,2,\ldots,m) \tag{22}$$

The Gibbs free energy of the mixture is an additive quantity

$$F = M_u \sum_{i=1}^{n} y_i f_i(p_i, T) = M_u \sum_{i=1}^{n} y_i \left[-RT \log_e Q_i(p_i, T) + h_{oi} \right] \tag{23}$$

where p_i is the partial pressure of species i. According to equations (2) and (3), Q is proportional to 1/p and equation (23) can be written as

$$F = M_u \sum_{i=1}^{n} y_i \left[-RT \log_e Q_i(p_o, T) + RT \log_e \frac{p}{p_o} + RT \log_e \frac{p_i}{p} + h_{oi} \right] \tag{24}$$

The ideal gas law for species i and Dalton's Law give

$$\frac{p_i}{p} = \frac{y_i}{\bar{y}} \tag{25}$$

where $\bar{y} = \sum_{i=1}^{n} y_i$. Thus the Gibbs free energy depends on temperature, pressure, and y_i as follows:

$$F = M_u \sum_{i=1}^{n} y_i \left[-RT \log_e Q_i(p_o, T) + h_{oi} + RT \log_e \frac{p}{p_o} + RT \log_e \frac{y_i}{\bar{y}} \right] \tag{26}$$

Notice that $Q_i(p_o, T)$ in equation (26) does not depend on p and needs to be computed only once for a given T.

The equilibrium concentrations are determined by minimizing F (eq. (26)) subject to the constraints (eqs. (22)). Since equation (26) is nonlinear, a numerical technique was used to minimize F. This technique, often called the RAND method or the method of White (derived in ref. 18), is widely used and has been shown to be equivalent to two other popular methods (ref. 24). An initial guess consistent with equations (22) must be made for y_i. A Taylor's series expansion of F about the initial y_i is then minimized to find a better set of y_i values. Iterations continue until the absolute value of each y_i changes by less than 10^{-7} between successive iterations. This criterion requires that the concentrations y_i of major species be accurate and is referred to as the absolute criterion. A relative criterion is also required in order to prevent termination of the iterations while a minor species is still changing by 0.1 of its previous value. Once the equilibrium set of y_i is known, the mixture properties can be calculated.

Equilibrium Mixture Properties

Density can readily be computed from the equation of state

$$\rho = \frac{p}{\bar{y}RT} \tag{27}$$

The enthalpy of the mixture is additive so that

$$H = M_u \sum_{i=1}^{n} y_i h_i \tag{28}$$

Entropy is related to F and H by

$$S = \frac{H - F}{T} \tag{29}$$

Molecular-weight ratio Z, sometimes called compressibility factor, is given by

$$Z = \frac{M_u}{M} = \bar{y}M_u \tag{30}$$

Electron number density N_e, the number of electrons per unit volume, is

$$N_e = N_o \frac{y_1}{\bar{y}} \frac{p}{RT} \tag{31}$$

where the subscript 1 refers to electrons. The Gibbs free energy F is given by equation (26).

RESULTS AND DISCUSSION

Thermodynamic properties were computed three times for each gas mixture, the diatomic species being treated by the direct-summation, modified, and rotating harmonic-oscillator methods (eqs. (6), (14), and (16)). Calculations were made for air, CO_2, and a Mars atmosphere. The composition of air is the same as that in references 1 and 8, except that neon has been omitted, and is 78.086 percent N_2, 20.947 percent O_2, 0.934 percent Ar, and 0.033 percent CO_2 by volume. The Mars atmosphere was based on the work of Kaplan reported in reference 25, and has the following composition: 25 percent N_2, 32 percent Ar, and 43 percent CO_2 by volume.

For N_2 and O_2 at atmospheric pressure ($p = p_o$), Gibbs free energy and enthalpy are presented in figures 2 to 5. Properties for all three mixtures and all three methods are given in tables IV to XIII. Comparisons of the modified results with other calculations are made for air in tables XIV to XVII. Finally, a sample Mollier diagram for the Mars atmosphere, computed by using the modified method, is given in figure 6. Detailed discussions of the tables and figures are given in the following sections.

Diatomic Species Properties

Ten diatomic species were considered: N_2, N_2^+, O_2, O_2^+, O_2^-, NO, NO^+, CO, CO^+, and CN. Comparisons of the direct-summation, modified, and rotating harmonic-oscillator results for N_2 and O_2 at $p = p_o$ are given in figures 2 to 5. These species were chosen because N_2 has a high dissociation energy and O_2 has a low dissociation energy. In figures 2 to 5 the property computed by the direct-summation method is presented in the upper graph. In the lower graph, the value of the quantity calculated by a given method minus that from the direct-summation method is plotted. This difference, denoted by $\Delta f_i/RT$ or $\Delta h_i/RT$, is plotted on a magnified scale. Differences are plotted for the rotating harmonic-oscillator, the modified, and Browne's (ref. 26) results. The results of Browne (ref. 26) are included since he essentially used the Mayer and Mayer method (ref. 14) and, in addition, all input constants for diatomic species used in the present work (tables I and III) are the same.

An important point illustrated by figures 2 to 5 is that for a given diatomic species, the difference between the modified and the direct-summation results is significant only at temperatures higher than that at which the species appreciably dissociates in a mixture of ideal gases. Thus, the modified-method results agree well with the direct-summation results for temperatures at which a given species concentration is not negligible. This behavior was observed for the 10 diatomic species considered for mixture pressures up to about 100 atmospheres.

Mixture Properties

Reciprocal molecular weight ratio, nondimensional enthalpy and entropy, logarithm of density ratio, and electron number density are given in tables IV to XIII for CO_2, the Mars atmosphere, and air. Three values are given for each mixture property to compare the three methods for treating the diatomic species. The following discussions are based on results for mixture pressures from $10^{-4}p_o$ to 10^2p_o. Above 10^2p_o, the assumption of a mixture of ideal gases breaks down (ref. 9). However, $10^{-4}p_o$ is not a lower limit on the validity of the assumptions but about the lower limit for which results for air have been independently checked.

The direct-summation method is considered to be the most accurate of the three methods for computing properties. Examination of results for temperatures from 1000° K to 15 000° K shows that properties computed by the modified method generally agree with those computed by the direct-summation method to well within 0.1 of 1 percent. Differences between the direct-summation and the rotating harmonic-oscillator method are generally within 1 percent except for electron number density which differs by almost 2 percent in some cases. Notice that the enthalpy of the CO_2 mixture at $p = 10p_o$ (table VI) differs more with choice of method than do the enthalpies of the other two mixtures. For example, at 3000° K the differences between the direct-summation and the rotating harmonic-oscillator methods for H/ZRT are about 0.07, 0.04, and 0.03 for CO_2, Mars, and air, respectively. These differences are clearly more meaningful than percent differences since H/ZRT passes through zero (changes sign) near 3000° K for CO_2 and Mars. The agreement of mixture properties regardless of method at 15 000° K is primarily due to the small quantity of diatomic species present for $p \leqq 10^2p_o$.

In all cases the absolute convergence criterion was used in the equilibrium composition calculation. In addition, the relative criterion was used in all three calculations for CO_2 and only in the modified calculations for Mars and air. Consequently, some electron number density values in the direct-summation and rotating harmonic-oscillator calculations for Mars and air were not comparable with the modified values. Those values were recomputed by using the relative criterion and the revised values are denoted by footnote a in tables XII and XIII.

None of the thermodynamic properties examined depend on the second partial derivative of the partition function with respect to temperature. Such properties include specific heat and would be expected to be more sensitive to the method of computation than those examined herein. A direct method for computing specific heats and related thermodynamic properties (using the present modified method for diatomic species) and the results obtained are given in reference 27.

Comparison With Other Results

The results in tables XIV to XVII are for air at various temperatures and two representative densities. Since the present paper takes temperature and pressure (not density) as independent variables, the data in tables XIV to XVII were generated by using the pressures computed by Browne. Comparisons of the present modified-method properties with those of Browne (ref. 8) and Gilmore (refs. 1 and 5) show agreement to within a few tenths of a percent except for electron number density. The present electron number density generally agrees with that of Browne (ref. 8) to about 0.5 percent. The 1.1-percent difference at $\log_{10} \frac{\rho}{\rho_0} = 0.000$ and $T = 3000^\circ$ K (table XVII) appears to be caused by numerical round-off error in the electron concentration variable y_1 which is small for high-density low-temperature conditions. The electron number density of Gilmore (refs. 1 and 5) disagrees with both the present results and those of Browne by as much as 8 percent in some cases. The fact that the present results agree better with those of Browne than with those of Gilmore is due to the use of thermochemical and spectroscopic constants (tables I to III) which are substantially the same as those used in the more recent work of Browne. Below about 10 000° K, the differences are primarily due to differences in diatomic species properties. At higher temperatures, atoms and atomic ions predominate and atomic-energy-level data become important. Properties above 15 000° K have been included for comparison but are felt to be approximate because of the uncertainties in data for high energy levels and the assumption of a mixture of ideal gases.

Since the rotating harmonic-oscillator results differ from the modified results by up to 2 percent, and the modified results agree to within 0.5 percent with Browne's virial results for air, the following conclusion seems evident. The present diatomic corrections account for most of the difference between the rotating harmonic-oscillator and the virial methodology results for the temperatures and pressures considered. This observation supports the use of the quadratic energy expresssion (eq. (8)) and the approximate vibrational-rotational cutoff criterion used for diatomic species.

Comparison of Three Mixtures

It is of interest to observe some of the similarities and differences among the three mixtures at a given temperature in tables IV to XIII. Reciprocal molecular weight ratio $1/Z$ is closest to unity for air and deviates most from unity for CO_2. This deviation occurs because undissociated CO_2 is triatomic whereas air is essentially diatomic. As dissociation takes place, the molecular weight of the CO_2 mixture changes more than that of air. Note that the enthalpy H/ZRT of CO_2 and the Mars atmosphere is negative at low temperatures since the CO_2 species has a negative enthalpy resulting from its negative heat of formation. The entropy S/R of the CO_2 mixture is seen to be higher than that of air or the Mars atmosphere at all temperatures considered. The density $\log_{10} \frac{\rho}{\rho_o}$ is about the same for all three gas mixtures, especially at low temperatures.

The CO_2 mixture at low temperatures has an order of magnitude smaller electron number density N_e than air and the Mars atmosphere. At high temperatures, however, the N_e values for all three mixtures are about the same. The N_e values are exceptionally close together for the highest temperature ($T = 15\ 000^\circ$ K) and the lowest pressure in the tables $\left(p = 10^{-3}p_o\right)$.

CONCLUSIONS

It is known that vibrational-rotational corrections for diatomic species must be considered in order to compute thermodynamic properties of mixtures of ideal gases accurately. Specific conclusions concerning these corrections are as follows:

1. The modified method results generally agree with those of the direct-summation method to well within 0.1 of 1 percent for the mixture properties examined.

2. The modified method requires about an order of magnitude less time than that used by the direct-summation method.

3. The rotating harmonic-oscillator results differ from the direct-summation results by up to 2 percent for mixture properties. However, specific heat and related quantities should differ by greater percentages.

4. Mixture property results for air using the modified method for diatomic species generally agree with Browne's virial methodology results and Gilmore's mixture-of-ideal-gases results to about 1/2 percent.

5. The present diatomic corrections account for most of the difference between the rotating harmonic-oscillator results and Browne's virial methodology results.

6. At high temperatures, the electron number density N_e is about the same for all three mixtures, especially for low pressures.

Langley Research Center,
National Aeronautics and Space Administration,
Langley Station, Hampton, Va., March 7, 1966.

APPENDIX

MODIFIED-METHOD PARTITION FUNCTION

The modified expression for $Q_{vib,rot}$ for diatomic species is derived in this appendix. Equations (6), (7), (8), and (10) can be combined and rearranged to yield

$$Q_{vib,rot} = \frac{1}{\sigma} \sum_{v=0}^{v_{max}} e^{-\frac{hc}{kT}\left[(\omega_e-\omega_e x_e)v-\omega_e x_e v^2\right]} \sum_{j=0}^{j(v)_{max}} (2j+1) e^{-\frac{hc}{kT}\left(B_e-\frac{1}{2}\alpha_e-\alpha_e v\right)j(j+1)} e^{\frac{hc}{kT}\frac{4B_e^3}{\omega_e^2}j^2(j+1)^2} \tag{A1}$$

In order to save computer time, it is desirable to replace the sum over j with an analytical expression. To this end, the upper limit on j was changed to infinity

$$j(v)_{max} = \infty \tag{A2}$$

and the smallest vibrational-rotational correction term was approximated by using the first two terms of the exponential expansion:

$$e^{\frac{hc}{kT}\frac{4B_e^3}{\omega_e^2}j^2(j+1)^2} \approx 1 + \frac{hc}{kT}\frac{4B_e^3}{\omega_e^2}j^2(j+1)^2 \tag{A3}$$

This expansion (used by Mayer and Mayer, ref. 14) was made to avoid divergence of the infinite summation. However, no other exponential expansions were made in the present modified method. The infinite (convergent) summation over j can be accurately approximated by using the Euler-Maclaurin summation formula for function $f(j)$:

$$\sum_{j=0}^{\infty} f(j) = \int_0^{\infty} f(j)dj + \frac{1}{2}f(0) - \frac{1}{12}f'(0) + \frac{1}{720}f'''(0) \dots \tag{A4}$$

as given in reference 14 (p. 152). Application of equation (A4) to the combination of equations (A1) to (A3), terms in negative powers of T being neglected, results in the expression

$$Q_{vib,rot} \approx \frac{1}{\sigma} \sum_{v=0}^{v_{max}} e^{-\frac{hc}{kT}\left[(\omega_e-\omega_e x_e)v-\omega_e x_e v^2\right]} \left[\frac{kT}{hc\left(B_e - \frac{\alpha_e}{2} - \alpha_e v\right)} + \frac{8B_e^3 k^2 T^2}{\omega_e^2 h^2 c^2 \left(B_e - \frac{\alpha_e}{2} - \alpha_e v\right)^3} + \frac{1}{3}\right] \tag{A5}$$

Terms in negative powers of T are neglected because they are small and inconsistent with the symmetry number (σ) approximation. Application of equation (A4) is valid only for values of v for which

$$B_e - \frac{\alpha_e}{2} - \alpha_e v > 0 \tag{A6}$$

The integral term in the Euler-Maclaurin summation formula will be infinite if this inequality does not hold for all values of v up to and including v_{max}. This inequality was found to hold for every electronic state of each diatomic species as given in table III with one exception: the $C^2\Sigma^+$ state of N_2^+. The value of v_{max} was reduced from 34 to 30 for that state in order to satisfy equation (A6).

When the enthalpy of a diatomic species is computed, the temperature derivative of $Q_{vib,rot}$ is needed. This derivative is obtained by taking the temperature derivative of equation (6), summing j to infinity by using the exponential expansion equation (A3), applying equation (A4) to the summation over j, and then neglecting terms in negative powers of T. The result is

$$\begin{aligned}\frac{\partial Q_{vib,rot}}{\partial T} \approx \frac{1}{\sigma T}\sum_{v=0}^{v_{max}}\Biggl\{&\frac{hc}{kT}\left[(\omega_e - \omega_e x_e)v - \omega_e x_e v^2\right]\left[\frac{kT}{hc\left(B_e - \frac{1}{2}\alpha_e - \alpha_e v\right)} + \frac{8B_e^3k^2T^2}{\omega_e^2h^2c^2\left(B_e - \frac{1}{2}\alpha_e - \alpha_e v\right)^3} + \frac{1}{3}\right]\\ &+ \frac{kT}{hc\left(B_e - \frac{1}{2}\alpha_e - \alpha_e v\right)} + \frac{16B_e^3k^2T^2}{\omega_e^2h^2c^2\left(B_e - \frac{1}{2}\alpha_e - \alpha_e v\right)^3} - \frac{384B_e^6k^3T^3}{\omega_e^4h^3c^3\left(B_e - \frac{1}{2}\alpha_e - \alpha_e v\right)^5}\Biggr\} e^{-\frac{hc}{kT}\left[(\omega_e - \omega_e x_e)v - \omega_e x_e v^2\right]}\end{aligned} \tag{A7}$$

REFERENCES

1. Gilmore, F. R.: Equilibrium Composition and Thermodynamic Properties of Air to 24,000° K. U.S. Air Force Proj. RAND Res. Mem. RM-1543, The RAND Corp., Aug. 24, 1955. (Available from ASTIA as AD 84052.)
2. Hilsenrath, Joseph; and Beckett, Charles W.: Tables of Thermodynamic Properties of Argon-Free Air to 15,000° K. AEDC-TN-56-12, Arnold Eng. Dev. Center, Sept. 1956. (Also available from ASTIA as Doc. No. AD-98974.)
3. Logan, J. G., Jr.; and Treanor, C. E.: Tables of Thermodynamic Properties of Air from 3000° K to 10,000° K at Intervals of 100° K. Rept. No. BE-1007-A-3, Cornell Aeron. Lab., Inc., Jan. 1957.
4. Hilsenrath, Joseph; Klein, Max; and Woolley, Harold W.: Tables of Thermodynamic Properties of Air Including Dissociation and Ionization from 1500° K to 15,000° K. AEDC-TR-59-20, U.S. Air Force, Dec. 1959. (Available from ASTIA as AD 229934.)
5. Gilmore, F. R.: Additional Values for the Equilibrium Composition and Thermodynamic Properties of Air. U.S. Air Force Proj. RAND Res. Mem. RM-2328, The RAND Corp., Dec. 30, 1959.
6. Hochstim, Adolf R.: Equilibrium Compositions, Thermodynamic and Normal Shock Properties of Air with Additives. Vol. 1., ZPh-122 (DA-04-495-ORD-3112 and -3383), Gen. Dyn./Convair, Dec. 1, 1961.
7. Hochstim, Adolf R.: Theoretical Calculation of Thermodynamic Properties of Air. Combustion and Propulsion Fifth AGARD Colloquium. – High-Temperature Phenomena, R. P. Hagerty; A. L. Jaumotte; O. Lutz; and S. S. Penner, eds., Pergamon Press, 1963, pp. 3-44.
8. Browne, W. G.: Thermodynamic Properties of the Earth's Atmosphere. Radiation and Space Phys. Tech. Mem. No. 2., Missile and Space Div., Gen. Elec. Co., Nov. 15, 1962.
9. Hilsenrath, Joseph; and Klein, Max: Tables of Thermodynamic Properties of Air in Chemical Equilibrium Including Second Virial Corrections from 1500° K to 15,000° K. AEDC-TDR-63-161, Arnold Eng. Develop. Center, Aug. 1963.
10. Hilsenrath, Joseph; and Klein, Max: Tables of Thermodynamic Properties of Air in Chemical Equilibrium Including Second Virial Corrections from 1500° K to 15,000° K. AEDC-TR-65-58, Arnold Eng. Dev. Center, U.S. Air Force, Mar. 1965.

11. Browne, William G.: Equilibrium Thermodynamic Properties of the Environment of Mars. Advanced Aerospace Phys. Tech. Mem. No. 2, Missile and Space Vehicle Dept., Gen. Elec. Co., Mar. 26, 1962.

12. Browne, William G.: Thermodynamic Properties of the Venusian Atmosphere – Part 1, Advanced Aerospace Phys. Tech. Mem. No. 13, pt. 1, Missile and Space Vehicle Dept., General Elec. Co., June 6, 1962.

13. Browne, William G.: Revised Thermodynamic Properties of the Venusian Atmosphere - Part 3, Advanced Aerospace Phys. Tech. Mem. No. 13, pt. 3, Missile and Space Vehicle Dept., General Elec. Co., June 6, 1962.

14. Mayer, Joseph E.; and Mayer, Maria Goeppert: Statistical Mechanics. John Wiley & Sons, Inc. (New York), c.1940.

15. Woolley, Harvey W.: Thermodynamic Functions for Molecular Oxygen in the Ideal Gas State. J. Res. Nat. Bur. Std., vol. 40, no. 2, Feb. 1948, pp. 163-168.

16. McBride, Bonnie J.; Heimel, Sheldon; Ehlers, Janet G.; and Gordon, Sanford: Thermodynamic Properties to 6,000° K for 210 Substances Involving the First 18 Elements. NASA SP-3001, 1963.

17. Glatt, Leonard; Belzer, Jack; Johnston, Herrick L.: Computation of Thermodynamic Properties of Gases from Spectra N_2. Tech. Rept. 316-9 (Contract N6-onr-225), Ohio State Univ. Res. Found., July 15, 1953.

18. White, W. B.; Johnson, S. M.; and Dantzig, G. B.: Chemical Equilibrium in Complex Mixtures. J. Chem. Phys., vol. 28, no. 5, May 1958, pp. 751-755.

19. Rocard, Y. (C. R. S. Manders, trans.): Thermodynamics. Sir Isaac Pitman and Sons, Ltd. (London), 1961.

20. Moore, Charlotte E.: Atomic Energy Levels. Vol. I-1H-23V, NBS Cir. 467, U.S. Dept. Com., June 15, 1949.

21. White, H. E.: Introduction to Atomic Spectra. McGraw-Hill Book Co., Inc., 1934.

22. Allison, Dennis O.: Calculation of Thermodynamic Properties of Gas Mixtures at High Temperatures. M.S. Thesis, Virginia Polytech. Inst., May 1965.

23. Herzberg, Gerhard: Molecular Spectra and Molecular Structure. I – Spectra of Diatomic Molecules. Second ed., D. Van Nostrand Co., Inc., c.1950.

24. Zeleznik, Frank J.; and Gordon, Sanford: An Analytical Investigation of Three General Methods of Calculating Chemical Equilibrium Compositions. NASA TN D-473, 1960.

25. Kaplan, Lewis D.; Münch, Guido; and Spinrad, Hyron: An Analysis of the Spectrum of Mars. Astrophys. J., vol. 139, no. 1, Jan. 1964, pp. 1-15.

26. Browne, William G.: Thermodynamic Properties of Some Diatomic and Linear Polyatomic Molecules. Eng. Phys. Tech. Memo No. 3, Missile and Space Vehicle Dept., Gen. Elec. Co.

27. Newman, Perry A.; and Allison, Dennis O.: Direct Calculation of Specific Heats and Related Thermodynamic Properties of Arbitrary Gas Mixtures With Tabulated Results. NASA TN D-3540, 1966.

28. Hodgman, Charles D.; Weast, Robert C.; and Selby, Samuel M., eds.: Handbook of Chemistry and Physics. Thirty-seventh ed., Chemical Rubber Publ. Co., c.1955.

29. Knight, Herbert T.; and Rink, John P.: Dissociation Energy of Cyanogen and Related Quantities by X-Ray Densitometry of Shock Waves. J. Chem. Phys., vol. 35, no. 1, July 1961, pp. 199-208.

30. Seman, Michael L.; and Branscomb, Lewis M.: Structure and Photodetachment Spectrum of the Atomic Carbon Negative Ion. Phys. Rev., Second ser., vol. 125, no. 5, Mar. 1, 1962, pp. 1602-1608.

31. Browne, W. G.: Comparison of Thermal Functions Generated for Species in the High Temperature Air System with Literature Values. Advanced Aerospace Phys. Tech. Mem. No. 10, Missile and Space Vehicle Dept., Gen. Elec. Co., May 28, 1962.

32. Schexnayder, Charles J., Jr.: Tabulated Values of Bond Dissociation Energies, Ionization Potentials, and Electron Affinities for Some Molecules Found in High-Temperature Chemical Reactions. NASA TN D-1791, 1963.

33. Browne, William G.: Thermodynamic Properties of the Species CN, C_2, C_3, C_2N_2, and C^-. Advanced Aerospace Phys. Tech. Mem. No. 9, Missile and Space Vehicle Dept., Gen. Elec. Co., May 14, 1962.

34. Mulliken, R. S.: The Energy Levels of the Nitrogen Molecule. The Threshold of Space, M. Zelikoff, ed., Pergamon Press, c.1957, pp. 169-179.

35. Beckett, Charles W.; and Haar, Lester: Thermodynamic Properties at High Temperatures: Ideal Gas Thermal Functions to 25,000 deg. K. for Diatomic Molecules, Oxygen, Nitrogen, Nitric Oxide, and Their Molecule Ions. Thermodynamic and Transport Properties of Fluids, Inst. Mech. Engrs. (London), 1958, pp. 27-33.

36. Herzberg, G.: Forbidden Transitions in Diatomic Molecules. III.- New $^1\Sigma_u^- \leftarrow {}^3\Sigma_g^-$ and $^3\Delta_u \leftarrow {}^3\Sigma_g^-$ Absorption Bands of the Oxygen Molecule. Can. J. Phys., vol. 31, no. 4, May 1953, pp. 657-669.

37. Konowalow, Daniel D.; and Hirschfelder, Joseph O.: Morse Potential Parameters for O-O, N-N, and N-O Interactions. Phys. Fluids, vol. 4, no. 5, May 1961, pp. 637-642.

38. Barrow, R. F.; and Miescher, E.: Fine Structure Analysis of NO Absorption Bands in the Schumann Region. Proc. Phys. Soc. (London), vol. 70, pt. 3, no. 447A, Mar. 1957, pp. 219-222.

39. Lagerqvist, A.; and Miescher, E.: Absorptionsspektrum des NO-Moleküls Feinstruktur-Analyse der δ- and β-Banden und homogene Störung $C^2\Pi$ - $B^2\Pi$. Helvetica Physica Acta, vol. XXXI, fasc. 3, 1958, pp. 221-262.

40. Miescher, E.: Rotationsanalyse der β'-Banden $\left(B'^2\Delta - X^2\pi\right)$ des NO-Moleküls. Helvetica Physica Acta, vol. 29, 1956, pp. 401-409.

41. Herzberg, Gerhard: Molecular Spectra and Molecular Structure. II.- Infrared and Raman Spectra of Polyatomic Molecules. D. Van Nostrand Co., Inc., c.1945.

TABLE I.- ATOMIC AND MOLECULAR CONSTANTS

[h_{oi} for CN is from ref. 29; h_{oi} for C^- is derived from ref. 30; h_{oi} for all other species is from ref. 31]

Species	Symmetry number, σ	M_i, gm/mole	h_{oi}, ergs/mole	D_o for ground state,[a] cm^{-1}
e^-	---	[b] 5.4847×10^{-4}	0	-----
N	---	14.008×10^0	4.70729×10^{12}	-----
N^+	---	14.007	18.72607	-----
N^{++}	---	14.007	47.28830	-----
O	---	16.000	2.46741	-----
O^+	---	15.999	15.60389	-----
O^{++}	---	15.999	49.47996	-----
O^-	---	16.001	1.05410	-----
C	---	12.011	7.11238	-----
C^+	---	12.010	17.97182	-----
C^{++}	---	12.010	41.49225	-----
C^-	---	12.012	5.89944	-----
Ar	---	39.944	0	-----
Ar^+	---	39.943	15.20235	-----
Ar^{++}	---	39.943	41.85170	-----
N_2	2	28.016	0	78 740
N_2^+	2	28.015	15.03336	70 420
O_2	2	32.000	0	41 260
O_2^+	2	31.999	11.62808	52 270
O_2^-	2	32.001	-.96232	37 480
NO	1	30.008	.89860	52 350
NO^+	1	30.007	9.82403	85 500
CO	1	28.011	-1.13813	89 610
CO^+	1	28.010	12.38367	68 000
CN	1	26.019	4.56056	60 900
CO_2	2	44.011	-3.93146	-----

[a] The ground-state dissociation energies D_o for diatomic species are from reference 32.

[b] M_i for e^- is from reference 28, page 3083.

TABLE II.- ATOMIC ENERGY LEVEL CONSTANTS

g_l	ν_l, cm^{-1}
Species e^-	
2	0
Species N	
4	0
10	19 225
6	28 840
12	83 330
6	86 180
12	88 140
2	93 582
20	94 800
12	95 500
4	96 752
10	96 810
6	97 800
10	99 660
18	104 000
34	104 700
56	105 000
22	106 600
16	107 200
16	107 600
54	109 600
12	109 860
106	110 350
132	111 600
136	112 200
6	112 310
68	112 820
30	112 910
2	113 600
10	113 900
14	117 000
Species N^+	
9	0
5	15 316
1	32 687
5	47 168
15	92 245
9	109 220
5	144 189
12	149 000
3	155 130
3	164 612
18	166 650
3	168 893
9	170 620
5	174 212
1	178 274
41	187 090
16	189 100
3	190 121
12	197 200
30	203 000
21	205 700
153	210 500
12	214 828
12	218 000
546	220 500
37	223 000
15	226 000
15	228 000
14	230 300
5	234 250
Species N^{++}	
6	0
12	57 280
10	101 026
2	131 044
6	145 920
4	186 802
10	203 078
2	221 302
6	230 407
6	245 690
10	267 242
12	287 650
6	297 210
2	301 088
32	310 500
4	314 224
22	317 550
14	320 288
10	321 040
30	329 000
22	333 300
22	336 290
20	339 550
48	343 000
24	348 000
32	364 000
12	368 620
22	374 000
52	379 000
2	380 700
Species O	
5	0
3	159
1	227
5	15 868
1	33 792
5	73 768
3	76 795
15	86 630
9	88 630
5	95 476
3	96 226
36	97 420
15	97 488
15	99 094
9	99 680
9	100 000
15	101 140
5	102 116
3	102 412
5	102 662
25	102 865
15	102 908
9	103 869
15	104 000
25	105 385
15	105 408
56	106 000
56	107 000
Species O^+	
4	0
10	26 820
6	40 465
12	120 000
10	165 990
12	185 400
6	189 000
2	195 710
2	203 942
42	207 600
26	212 800
2	226 851
24	230 000
80	232 700
16	233 900
18	239 600
40	245 500
20	248 000
6	250 300
32	251 900
44	254 000
84	255 500
116	256 000
18	258 100
10	259 300
72	261 500
166	265 500
134	270 000
142	276 500
24	283 000
Species O^{++}	
9	0
5	20 271
1	43 184
5	60 312
15	120 050
9	142 383
5	187 049
3	197 087
3	210 459
12	270 000
9	283 900
26	294 000
14	303 000
1	313 801
50	327 000
10	332 000
15	338 700
1	343 303
9	350 200
12	357 500
46	365 000
48	370 500
158	380 000
62	394 000
90	398 000
558	403 400
72	425 000
311	430 000
48	438 000
15	442 710
Species O^-	
6	0
Species C	
9	0
5	10 194
1	21 648
5	33 735
9	60 360

TABLE II.- ATOMIC ENERGY LEVEL CONSTANTS – Concluded

g_l	ν_l, cm^{-1}
Species C	
3	61 982
15	64 090
3	68 858
15	69 700
3	70 744
9	71 365
5	72 611
1	73 976
9	75 256
5	77 681
9	78 130
21	78 230
18	78 320
10	78 600
9	79 318
18	80 400
12	81 200
5	81 770
1	82 252
53	83 800
103	84 000
30	84 940
6	85 400
503	86 400
19	86 500
Species C^+	
6	0
12	43 030
10	74 931
2	96 494
6	101 800
6	110 650
2	114 900
2	116 538
14	119 400
6	131 731
Species C^+	
12	135 800
20	136 000
4	142 024
10	145 551
10	150 465
2	157 234
6	162 522
12	167 000
10	168 124
20	168 900
2	173 348
6	175 293
16	178 350
32	179 000
26	182 000
4	184 689
12	186 450
10	188 600
30	195 500
20	196 572
Species C^{++}	
1	0
9	52 360
3	102 351
9	137 420
5	145 875
1	182 520
3	238 161
1	247 170
3	258 931
9	259 662
15	269 960
5	276 843
15	309 100
1	311 721
12	318 700
Species C^{++}	
61	322 550
5	324 212
12	328 000
31	333 000
15	337 626
13	340 000
7	341 368
3	343 256
30	345 000
60	346 600
7	348 000
12	376 600
18	381 500
13	384 345
34	386 000
Species C^-	
6	0
Species Ar	
1	0
5	93 144
3	93 751
1	94 554
3	95 400
3	104 102
12	105 500
8	106 150
1	107 054
8	107 220
4	108 000
4	111 280
16	111 750
8	112 900
20	113 550
16	114 750
8	115 000
3	116 660
Species Ar	
12	116 960
8	117 170
1	117 563
16	118 530
36	119 300
56	120 250
20	120 700
32	121 750
36	122 200
56	122 700
20	123 500
28	124 136
Species Ar^+	
6	0
2	108 723
20	132 400
12	134 800
6	138 600
28	142 700
6	145 200
12	147 650
10	148 750
10	150 000
12	155 160
30	158 300
12	161 000
2	167 309
14	170 600
26	173 000
38	174 800
6	179 700
40	183 000
60	186 000
62	190 200
34	192 200
120	194 000
84	196 000
Species Ar^+	
48	200 000
18	205 000
6	208 593
220	210 000
50	215 000
70	220 000
Species Ar^{++}	
5	0
3	1 112
1	1 570
5	14 010
1	33 267
9	114 400
10	128 000
28	144 650
15	156 950
5	174 375
15	182 000
75	189 500
15	196 600
5	200 000
18	204 700
21	208 300
27	210 800
33	214 500
46	224 500
9	231 500
5	235 000
26	240 000
50	246 036
91	251 000
24	258 000
127	270 000
121	278 500
116	282 000
111	286 000
524	302 000

TABLE III.- MOLECULAR ENERGY LEVEL CONSTANTS*

[All constants were assembled by W. G. Browne in refs. 26 and 33. His source references are given in this table for convenience.]

Electronic state	g_l	ν_l, cm^{-1}	B_e, cm^{-1}	α_e, cm^{-1}	ω_e, cm^{-1}	$\omega_e x_e$, cm^{-1}	Reference
			Species N_2				
$X^1\Sigma_g^+$	1	0	1.998	0.017	2358.07	14.19	34
$A^3\Sigma_u^+$	3	49 757	1.440	.013	1460.37	13.89	34
$B^3\Pi_g$	6	59 314	1.638	.0184	1734.11	14.47	34
$a^1\Pi_g$	2	68 953	1.6182	.0183	1693.70	13.83	34
$a'^1\Sigma_u^-$	1	70 700	1.480	.0164	1530.00	12.00	34
$C^3\Pi_u$	6	87 984	1.8258	.0197	2035.10	17.08	34
			Species N_2^+				
$X^2\Sigma_g^+$	2	0	1.9322	0.0202	2207.23	16.22	35
$A^2\Pi_u$	4	9 020	1.722	.0180	1902.84	14.91	35, 1
$B^2\Sigma_u^+$	2	25 570	2.083	.0195	2419.84	23.19	35, 23
$C^2\Sigma^+$	2	64 550	1.650	.0500	2050.00	14.92	35, 23, 26
			Species O_2				
$X^3\Sigma_g^-$	3	0	1.4457	0.0158	1580.36	12.07	23
$a^1\Delta_g$	2	7 882.4	1.4264	.0171	1509.30	12.90	23
$b^1\Sigma_g^+$	1	13 120.9	1.4004	.0182	1432.69	13.95	23
$A^3\Sigma_u^+$	3	35 713.0	1.0500	.0357	819.00	22.50	23, 26
$^1\Sigma_u^-$	1	36 212.7	.8260	.0205	650.40	17.03	36
$B^3\Sigma_u^-$	3	49 363.1	.8190	.0110	700.36	8.00	23
			Species O_2^+				
$X^2\Pi_g$	4	0	1.6722	0.0198	1876.40	16.53	23
$a^4\Pi_u$	8	31 500	1.1047	.0158	1035.69	10.39	35, 23
$A^2\Pi_u$	4	38 300	1.0617	.0191	900.00	13.40	35, 23
$b^4\Sigma_g^-$	4	48 100	1.2873	.0221	1196.77	17.09	35, 23
			Species O_2^-				
$^2\Pi_g$	4	0	1.200	0.016	1300.00	14.00	1
$^4\Sigma_u^-$	4	13 400	.970	.017	990.00	15.00	1
$^2\Delta_u$	4	24 200	.920	.027	560.00	13.00	1

*The following relations were used when necessary to convert from constants given in the references to the constants in this table:

From reference 14,

$$\omega_o = \omega_e - \omega_e x_e$$

$$B_o = B_e - \frac{1}{2}\alpha_e$$

From reference 23,

$$\nu_l = (\nu_e)_l + \left(\frac{1}{2}\omega_e - \frac{1}{4}\omega_e x_e\right)_l - \left(\frac{1}{2}\omega_e - \frac{1}{4}\omega_e x_e\right)_{\text{ground state}}$$

TABLE III.- MOLECULAR ENERGY LEVEL CONSTANTS - Concluded

Electronic state	g_l	ν_l, cm^{-1}	B_e, cm^{-1}	α_e, cm^{-1}	ω_e, cm^{-1}	$\omega_e x_e$, cm^{-1}	Reference
Species NO							
$X^2\Pi_{1/2}$	2	0	1.7046	0.0178	1904.03	13.97	23
$X^2\Pi_{3/2}$	2	120.9	1.7046	.0178	1903.68	13.97	23
$A^2\Sigma^+$	2	44 200	1.9972	.0193	2374.80	16.46	35, 37, 38
$B^2\Pi$	4	45 440	1.1260	.0152	1037.68	7.603	23
$D^2\Sigma^+$	2	53 290	2.0026	.0218	2323.90	22.885	35, 37, 38
$C^2\Pi$	4	52 376	2.0020	.0300	2395.00	15.000	37, 39
$E^2\Sigma^+$	2	60 860	1.9863	.0182	2373.60	15.850	23
$B'^2\Delta$	4	60 020	1.3300	.0190	1216.60	15.880	37, 40
Species NO^+							
$X^1\Sigma^+$	1	0	2.002	0.0202	2377.10	16.35	1
$^3\Pi$	6	39 982	1.680	.0190	1740.00	14.50	1
$^3\Sigma^+$	3	58 523	1.330	.0160	1220.00	9.50	1
$^3\Pi$	6	72 384	1.260	.0170	1140.00	7.60	1
$A^1\Pi$	2	73 083.8	1.587	.0240	1608.90	23.30	1
Species CO							
$X^1\Sigma^+$	1	0	1.9313	0.01748	2170.21	13.461	23
$a^3\Pi_r$	6	48 473.9	1.6810	.01930	1739.25	14.470	23
$a'^3\Sigma^+$	3	55 380.0	1.3310	.01600	1218.00	9.500	23
$d^3\Pi_i$	6	61 784.6	1.2615	.01700	1137.79	7.624	23
$A^1\Pi$	2	64 746.5	1.6116	.02229	1515.61	17.2505	23
$b^3\Sigma^+$	3	83 831.0	2.0750	.03300	2198.00	13.476	23, 26
$B^1\Sigma^+$	1	86 917.8	1.9610	.02700	2082.07	12.092	23, 26
Species CO^+							
$X^2\Sigma^+$	2	0	1.9772	0.01896	2214.24	15.164	23
$A^2\Pi_i$	4	20 407.5	1.5894	.01942	1562.06	13.530	23
$B^2\Sigma^+$	2	45 633.5	1.7999	.03025	1734.18	27.927	23
Species CN							
$X^2\Sigma^+$	2	0	1.8996	0.01735	2068.705	13.144	23
$A^2\Pi_i$	4	9 114.59	1.7165	.01746	1814.430	12.883	23
$B^2\Sigma^+$	2	25 797.85	1.9701	.02215	2164.130	20.250	23
Species CO_2							
$^1\Sigma$	1	0	0.3906	0.0022	667.33	0	41, 26
					667.33	0	26
					1342.86	0	26
					2349.30	0	26

TABLE IV.- RECIPROCAL MOLECULAR WEIGHT RATIO 1/Z AT $p = 10p_o$

T, °K	Reciprocal molecular weight ratio for CO_2 determined by –			Reciprocal molecular weight ratio for Mars atmosphere determined by –			Reciprocal molecular weight ratio for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	0.99999	0.99999	0.99999	1.00000	0.99999	1.00000	1.00000	1.00000	1.00000
1 500	.99991	.99990	.99991	.99995	.99994	.99995	1.00000	.99999	1.00000
2 000	.99648	.99648	.99653	.99793	.99792	.99795	.99995	.99994	.99995
2 500	.96889	.96890	.96946	.98168	.98168	.98200	.99898	.99898	.99897
3 000	.88423	.88426	.88625	.93227	.93228	.93337	.99245	.99244	.99231
3 500	.75899	.75903	.76146	.85943	.85944	.86059	.97070	.97070	.97010
4 000	.64610	.64612	.64672	.79175	.79175	.79175	.93003	.93003	.92868
4 500	.56697	.56697	.56613	.74368	.74368	.74296	.88675	.88674	.88513
5 000	.52565	.52565	.52484	.71841	.71840	.71776	.85725	.85725	.85594
5 500	.50956	.50956	.50912	.70553	.70553	.70502	.83717	.83718	.83611
6 000	.50348	.50348	.50324	.69463	.69463	.69409	.81616	.81617	.81503
6 500	.49928	.49929	.49904	.67894	.67893	.67809	.78669	.78668	.78513
7 000	.49057	.49057	.48993	.65204	.65203	.65044	.74483	.74482	.74251
7 500	.46928	.46927	.46763	.61026	.61023	.60760	.69182	.69179	.68865
8 000	.43319	.43316	.43048	.56186	.56182	.55875	.63513	.63509	.63149
8 500	.39401	.39397	.39119	.52201	.52198	.51943	.58539	.58536	.58203
9 000	.36457	.36454	.36247	.49675	.49674	.49505	.54944	.54942	.54687
9 500	.34679	.34678	.34549	.48250	.48249	.48150	.52687	.52686	.52515
10 000	.33653	.33653	.33578	.47403	.47403	.47346	.51334	.51334	.51226
11 000	.32469	.32469	.32444	.46250	.46250	.46229	.49815	.49816	.49774
12 000	.31451	.31451	.31442	.45024	.45025	.45016	.48583	.48584	.48566
13 000	.30239	.30240	.30236	.43405	.43405	.43401	.47014	.47015	.47007
14 000	.28783	.28784	.28782	.41316	.41316	.41314	.44909	.44910	.44905
15 000	.27133	.27134	.27133	.38816	.38816	.38815	.42272	.42273	.42271

TABLE V.- RECIPROCAL MOLECULAR WEIGHT RATIO 1/Z AT $p = 10^{-3}p_o$

T, °K	Reciprocal molecular weight ratio for CO_2 determined by –			Reciprocal molecular weight ratio for Mars atmosphere determined by –			Reciprocal molecular weight ratio for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	0.99999	0.99999	0.99998	1.00000	0.99999	1.00000	1.00000	1.00000	1.00000
1 500	.99817	.99818	.99819	.99896	.99895	.99896	.99997	.99996	.99997
2 000	.93099	.93100	.93180	.96020	.96020	.96065	.99527	.99526	.99522
2 500	.66194	.66196	.66251	.79851	.79851	.79863	.92427	.92427	.92350
3 000	.51185	.51185	.51163	.70670	.70670	.70656	.83703	.83702	.83674
3 500	.50067	.50067	.50065	.69919	.69919	.69916	.82616	.82616	.82608
4 000	.50000	.50000	.50000	.69166	.69165	.69154	.80928	.80929	.80904
4 500	.49732	.49732	.49723	.66188	.66185	.66134	.74550	.74550	.74445
5 000	.46196	.46195	.46085	.58169	.58168	.58020	.61895	.61894	.61708
5 500	.37493	.37492	.37359	.50000	.49999	.49906	.52994	.52994	.52905
6 000	.33694	.33694	.33660	.47417	.47416	.47396	.50679	.50680	.50658
6 500	.32519	.32519	.32512	.46424	.46424	.46420	.50084	.50084	.50078
7 000	.31383	.31383	.31381	.45222	.45222	.45221	.49554	.49554	.49552
7 500	.29799	.29799	.29799	.43486	.43486	.43486	.48582	.48582	.48582
8 000	.27885	.27885	.27885	.41303	.41303	.41303	.46797	.46798	.46797
8 500	.25935	.25936	.25935	.38748	.38748	.38747	.43903	.43903	.43903
9 000	.24007	.24008	.24007	.35690	.35690	.35690	.39903	.39904	.39903
9 500	.22015	.22015	.22015	.32250	.32251	.32250	.35369	.35370	.35369
10 000	.20133	.20133	.20133	.29038	.29038	.29038	.31309	.31310	.31309
11 000	.17748	.17748	.17748	.25236	.25236	.25236	.26821	.26821	.26821
12 000	.16967	.16967	.16967	.24103	.24103	.24103	.25560	.25560	.25560
13 000	.16755	.16755	.16755	.23812	.23812	.23812	.25245	.25245	.25245
14 000	.16675	.16675	.16675	.23706	.23706	.23706	.25154	.25154	.25154
15 000	.16573	.16573	.16573	.23560	.23560	.23559	.25105	.25105	.25105

TABLE VI.- NONDIMENSIONAL ENTHALPY H/ZRT AT $p = 10p_o$

T, °K	Nondimensional enthalpy for CO_2 determined by –			Nondimensional enthalpy for Mars atmosphere determined by –			Nondimensional enthalpy for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	-42.145	-42.146	-42.145	-16.417	-16.417	-16.418	3.6305	3.6305	3.6248
1 500	-25.833	-25.833	-25.834	-9.3646	-9.3646	-9.3669	3.7996	3.7995	3.7883
2 000	-17.428	-17.428	-17.431	-5.7131	-5.7132	-5.7179	3.9605	3.9602	3.9435
2 500	-11.420	-11.420	-11.444	-3.0679	-3.0681	-3.0839	4.1343	4.1338	4.1119
3 000	-5.6978	-5.6987	-5.7719	-.5089	-.5095	-.5478	4.3766	4.3760	4.3508
3 500	-.7837	-.7850	-.8709	1.7006	1.6998	1.6572	4.7518	4.7511	4.7275
4 000	2.3635	2.3624	2.3181	3.1398	3.1391	3.1144	5.1963	5.1956	5.1771
4 500	4.0026	4.0018	3.9862	3.8837	3.8830	3.8673	5.4999	5.4992	5.4806
5 000	4.6269	4.6260	4.6097	4.1656	4.1649	4.1469	5.6036	5.6028	5.5797
5 500	4.7607	4.7596	4.7365	4.2777	4.2768	4.2563	5.6543	5.6533	5.6281
6 000	4.7511	4.7499	4.7223	4.4007	4.3997	4.3799	5.7818	5.7808	5.7579
6 500	4.7571	4.7557	4.7281	4.6370	4.6360	4.6227	6.0502	6.0492	6.0343
7 000	4.9192	4.9178	4.9009	5.0822	5.0814	5.0846	6.4680	6.4672	6.4654
7 500	5.4042	5.4032	5.4143	5.7605	5.7602	5.7861	6.9789	6.9785	6.9914
8 000	6.1883	6.1881	6.2287	6.4690	6.4692	6.5065	7.4674	7.4674	7.4903
8 500	6.9307	6.9310	6.9779	6.9404	6.9407	6.9723	7.8136	7.8138	7.8378
9 000	7.3586	7.3591	7.3933	7.1225	7.1228	7.1426	7.9701	7.9703	7.9888
9 500	7.4931	7.4935	7.5135	7.1213	7.1215	7.1322	7.9754	7.9756	7.9875
10 000	7.4675	7.4677	7.4784	7.0424	7.0426	7.0482	7.8979	7.8982	7.9051
11 000	7.2814	7.2815	7.2845	6.8560	6.8561	6.8577	7.6835	7.6836	7.6858
12 000	7.1207	7.1208	7.1216	6.7409	6.7410	6.7414	7.5204	7.5205	7.5213
13 000	7.0382	7.0383	7.0386	6.7252	6.7252	6.7254	7.4512	7.4513	7.4515
14 000	7.0279	7.0279	7.0280	6.8014	6.8014	6.8015	7.4719	7.4719	7.4720
15 000	7.0701	7.0701	7.0701	6.9438	6.9438	6.9438	7.5575	7.5575	7.5575

TABLE VII.- NONDIMENSIONAL ENTHALPY H/ZRT AT $p = 10^{-3}p_o$

T, °K	Nondimensional enthalpy for CO_2 determined by –			Nondimensional enthalpy for Mars atmosphere determined by –			Nondimensional enthalpy for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	-42.146	-42.146	-42.145	-16.417	-16.417	-16.418	3.6305	3.6305	3.6248
1 500	-25.711	-25.711	-25.712	-9.3104	-9.3105	-9.3133	3.8007	3.8005	3.7894
2 000	-14.090	-14.090	-14.135	-4.2294	-4.2297	-4.2528	4.0851	4.0848	4.0697
2 500	.4408	.4400	.4007	2.3606	2.3602	2.3429	5.6472	5.6470	5.6448
3 000	5.6320	5.6317	5.6236	4.7162	4.7159	4.7063	6.8135	6.8132	6.8018
3 500	5.6128	5.6123	5.5967	4.6951	4.6948	4.6810	6.5580	6.5577	6.5410
4 000	5.3698	5.3693	5.3507	4.7947	4.7943	4.7815	6.6601	6.6597	6.6462
4 500	5.2976	5.2970	5.2803	5.5822	5.5822	5.5823	7.8841	7.8838	7.8910
5 000	6.6559	6.6556	6.6846	7.7451	7.7451	7.7800	10.179	10.179	10.209
5 500	9.7445	9.7447	9.7896	9.6303	9.6305	9.6540	11.265	11.265	11.280
6 000	10.527	10.527	10.537	9.7505	9.7505	9.7554	10.993	10.993	10.996
6 500	10.337	10.337	10.339	9.4809	9.4809	9.4818	10.511	10.511	10.511
7 000	10.187	10.187	10.187	9.3233	9.3232	9.3235	10.140	10.140	10.140
7 500	10.211	10.211	10.212	9.3340	9.3340	9.3341	9.9662	9.9662	9.9663
8 000	10.350	10.350	10.350	9.4840	9.4839	9.4840	10.047	10.047	10.047
8 500	10.521	10.521	10.521	9.7714	9.7714	9.7714	10.409	10.408	10.409
9 000	10.731	10.731	10.731	10.227	10.227	10.227	10.995	10.995	10.995
9 500	10.997	10.996	10.997	10.778	10.778	10.778	11.632	11.632	11.632
10 000	11.226	11.226	11.226	11.230	11.230	11.230	12.086	12.086	12.086
11 000	11.216	11.216	11.216	11.378	11.378	11.378	12.126	12.126	12.126
12 000	10.751	10.751	10.751	10.910	10.910	10.910	11.569	11.569	11.569
13 000	10.209	10.209	10.209	10.346	10.346	10.346	10.942	10.942	10.942
14 000	9.7215	9.7215	9.7214	9.8391	9.8391	9.8391	10.373	10.373	10.373
15 000	9.3373	9.3373	9.3373	9.4445	9.4445	9.4445	9.8831	9.8831	9.8831

TABLE VIII.- NONDIMENSIONAL ENTROPY S/R AT $p = 10p_o$

T, °K	Nondimensional entropy for CO_2 determined by –			Nondimensional entropy for Mars atmosphere determined by –			Nondimensional entropy for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	30.066	30.066	30.066	26.471	26.471	26.469	26.030	26.030	26.020
1 500	32.810	32.810	32.810	28.388	28.388	28.384	27.704	27.703	27.684
2 000	34.973	34.972	34.971	29.877	29.877	29.870	28.980	28.980	28.951
2 500	37.408	37.408	37.388	31.485	31.485	31.466	30.060	30.059	30.021
3 000	41.071	41.069	40.992	33.720	33.720	33.670	31.107	31.107	31.061
3 500	45.899	45.896	45.763	36.355	36.354	36.285	32.306	32.304	32.259
4 000	50.769	50.767	50.658	38.743	38.742	38.688	33.695	33.694	33.656
4 500	54.813	54.811	54.752	40.547	40.546	40.504	35.006	35.005	34.968
5 000	57.404	57.402	57.341	41.708	41.706	41.659	36.014	36.012	35.966
5 500	58.815	58.812	58.729	42.538	42.537	42.483	36.864	36.862	36.810
6 000	59.727	59.724	59.624	43.349	43.347	43.292	37.795	37.792	37.742
6 500	60.576	60.572	60.468	44.368	44.366	44.322	38.990	38.988	38.950
7 000	61.796	61.792	61.714	45.870	45.868	45.859	40.587	40.585	40.577
7 500	64.019	64.017	64.025	48.105	48.105	48.159	42.636	42.635	42.669
8 000	67.615	67.614	67.749	50.854	50.855	50.963	45.009	45.009	45.087
8 500	71.885	71.887	72.097	53.391	53.392	53.503	47.361	47.362	47.461
9 000	75.564	75.565	75.754	55.226	55.227	55.308	49.317	49.318	49.408
9 500	78.120	78.121	78.248	56.436	56.436	56.485	50.752	50.753	50.817
10 000	79.828	79.829	79.904	57.294	57.294	57.321	51.785	51.785	51.826
11 000	82.195	82.195	82.220	58.676	58.675	58.685	53.293	53.293	53.309
12 000	84.368	84.367	84.377	60.117	60.117	60.121	54.692	54.692	54.698
13 000	86.837	86.836	86.840	61.856	61.856	61.858	56.312	56.312	56.315
14 000	89.742	89.741	89.743	64.005	64.005	64.006	58.302	58.301	58.303
15 000	93.120	93.119	93.120	66.614	66.613	66.614	60.729	60.729	60.730

TABLE IX.- NONDIMENSIONAL ENTROPY S/R AT $p = 10^{-3}p_o$

T, °K	Nondimensional entropy for CO_2 determined by –			Nondimensional entropy for Mars atmosphere determined by –			Nondimensional entropy for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	39.277	39.277	39.277	35.681	35.682	35.679	35.240	35.240	35.230
1 500	42.104	42.104	42.103	37.646	37.647	37.642	36.915	36.915	36.896
2 000	46.753	46.752	46.714	40.530	40.530	40.503	38.344	38.343	38.316
2 500	60.765	60.763	60.685	47.668	47.667	47.633	41.423	41.423	41.411
3 000	72.395	72.394	72.362	52.367	52.367	52.342	44.808	44.808	44.783
3 500	74.344	74.342	74.287	53.447	53.447	53.411	45.849	45.847	45.812
4 000	75.338	75.337	75.271	54.568	54.567	54.531	47.207	47.205	47.173
4 500	76.502	76.500	76.435	56.952	56.952	56.940	50.627	50.626	50.632
5 000	81.504	81.502	81.568	62.935	62.935	63.015	57.888	57.887	57.974
5 500	94.987	94.987	95.185	70.459	70.459	70.537	64.533	64.532	64.593
6 000	102.79	102.79	102.85	73.518	73.518	73.537	66.855	66.854	66.870
6 500	105.87	105.87	105.88	75.018	75.018	75.022	67.859	67.859	67.862
7 000	108.91	108.91	108.92	76.729	76.729	76.730	68.868	68.868	68.869
7 500	113.01	113.01	113.02	79.024	79.024	79.025	70.330	70.329	70.330
8 000	118.16	118.16	118.16	81.951	81.951	81.952	72.633	72.633	72.634
8 500	123.96	123.96	123.96	85.663	85.662	85.663	76.234	76.233	76.234
9 000	130.53	130.53	130.53	90.633	90.633	90.634	81.536	81.535	81.536
9 500	138.33	138.33	138.33	97.070	97.069	97.070	88.496	88.494	88.496
10 000	146.85	146.85	146.85	104.17	104.17	104.17	96.046	96.044	96.046
11 000	160.02	160.02	160.02	114.63	114.63	114.63	106.71	106.71	106.71
12 000	165.73	165.72	165.73	118.77	118.77	118.77	110.73	110.73	110.73
13 000	168.28	168.27	168.28	120.51	120.51	120.51	112.36	112.36	112.36
14 000	170.06	170.06	170.06	121.71	121.71	121.71	113.39	113.39	113.39
15 000	172.05	172.05	172.05	123.11	123.10	123.11	114.30	114.29	114.30

TABLE X.- LOGARITHM OF DENSITY RATIO $\log_{10} \frac{\rho}{\rho_o}$ AT $p = 10p_o$

T, °K	Logarithm of density ratio for CO_2 determined by –			Logarithm of density ratio for Mars atmosphere determined by –			Logarithm of density ratio for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	0.43642	0.43640	0.43642	0.43642	0.43640	0.43642	0.43642	0.43640	0.43642
1 500	.26029	.26027	.26029	.26031	.26028	.26031	.26033	.26031	.26033
2 000	.13386	.13384	.13389	.13449	.13447	.13450	.13537	.13535	.13537
2 500	.02476	.02474	.02502	.03046	.03043	.03060	.03804	.03802	.03804
3 000	-.09413	-.09414	-.09313	-.07115	-.07118	-.07064	-.04399	-.04401	-.04405
3 500	-.22740	-.22741	-.22599	-.17343	-.17345	-.17284	-.12056	-.12058	-.12082
4 000	-.35533	-.35535	-.35491	-.26704	-.26707	-.26704	-.19714	-.19716	-.19776
4 500	-.46322	-.46325	-.46387	-.34539	-.34543	-.34582	-.26898	-.26901	-.26978
5 000	-.54184	-.54187	-.54251	-.40617	-.40620	-.40656	-.32943	-.32946	-.33010
5 500	-.59673	-.59676	-.59711	-.45542	-.45545	-.45573	-.38112	-.38114	-.38167
6 000	-.63974	-.63977	-.63994	-.49997	-.50000	-.50030	-.42994	-.42997	-.43055
6 500	-.67813	-.67816	-.67835	-.54465	-.54469	-.54519	-.48067	-.48071	-.48154
7 000	-.71796	-.71800	-.71853	-.59439	-.59443	-.59546	-.53661	-.53665	-.53797
7 500	-.76719	-.76724	-.76872	-.65311	-.65317	-.65501	-.59864	-.59869	-.60063
8 000	-.82998	-.83004	-.83270	-.71703	-.71709	-.71944	-.66380	-.66385	-.66629
8 500	-.89748	-.89755	-.90059	-.77530	-.77536	-.77746	-.72554	-.72559	-.72804
9 000	-.95603	-.95609	-.95853	-.82167	-.82171	-.82315	-.77789	-.77794	-.77992
9 500	-1.0012	-1.0013	-1.0028	-.85779	-.85783	-.85870	-.81959	-.81963	-.82101
10 000	-1.0365	-1.0366	-1.0375	-.88775	-.88779	-.88828	-.85316	-.85320	-.85408
11 000	-1.0935	-1.0935	-1.0938	-.93985	-.93988	-.94004	-.90759	-.90762	-.90796
12 000	-1.1451	-1.1451	-1.1452	-.98930	-.98933	-.98937	-.95626	-.95629	-.95641
13 000	-1.1969	-1.1970	-1.1970	-1.0400	-1.0400	-1.0400	-1.0053	-1.0053	-1.0053
14 000	-1.2505	-1.2506	-1.2506	-1.0936	-1.0936	-1.0936	-1.0574	-1.0574	-1.0574
15 000	-1.3061	-1.3062	-1.3062	-1.1506	-1.1507	-1.1507	-1.1136	-1.1136	-1.1136

TABLE XI.- LOGARITHM OF DENSITY RATIO $\log_{10} \frac{\rho}{\rho_o}$ AT $p = 10^{-3}p_o$

T, °K	Logarithm of density ratio for CO_2 determined by –			Logarithm of density ratio for Mars atmosphere determined by –			Logarithm of density ratio for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	-3.5636	-3.5636	-3.5636	-3.5636	-3.5636	-3.5636	-3.5636	-3.5636	-3.5636
1 500	-3.7405	-3.7405	-3.7405	-3.7401	-3.7401	-3.7401	-3.7397	-3.7397	-3.7397
2 000	-3.8957	-3.8957	-3.8953	-3.8822	-3.8823	-3.8820	-3.8667	-3.8667	-3.8667
2 500	-4.1407	-4.1407	-4.1403	-4.0592	-4.0593	-4.0592	-3.9957	-3.9957	-3.9961
3 000	-4.3316	-4.3316	-4.3317	-4.1915	-4.1915	-4.1915	-4.1180	-4.1180	-4.1181
3 500	-4.4081	-4.4081	-4.4081	-4.2630	-4.2631	-4.2631	-4.1906	-4.1906	-4.1906
4 000	-4.4667	-4.4667	-4.4667	-4.3257	-4.3258	-4.3258	-4.2575	-4.2576	-4.2577
4 500	-4.5201	-4.5202	-4.5202	-4.3960	-4.3960	-4.3964	-4.3443	-4.3444	-4.3449
5 000	-4.5979	-4.5980	-4.5990	-4.4978	-4.4979	-4.4990	-4.4709	-4.4709	-4.4722
5 500	-4.7300	-4.7300	-4.7315	-4.6050	-4.6050	-4.6058	-4.5797	-4.5797	-4.5804
6 000	-4.8142	-4.8142	-4.8146	-4.6658	-4.6658	-4.6660	-4.6369	-4.6369	-4.6371
6 500	-4.8643	-4.8644	-4.8644	-4.7097	-4.7098	-4.7098	-4.6768	-4.6768	-4.6768
7 000	-4.9120	-4.9120	-4.9120	-4.7533	-4.7534	-4.7533	-4.7136	-4.7136	-4.7136
7 500	-4.9644	-4.9645	-4.9644	-4.8003	-4.8003	-4.8003	-4.7521	-4.7522	-4.7522
8 000	-5.0213	-5.0213	-5.0213	-4.8507	-4.8507	-4.8507	-4.7964	-4.7965	-4.7964
8 500	-5.0791	-5.0791	-5.0791	-4.9047	-4.9048	-4.9047	-4.8505	-4.8505	-4.8505
9 000	-5.1375	-5.1375	-5.1375	-4.9653	-4.9653	-4.9653	-4.9168	-4.9168	-4.9168
9 500	-5.1986	-5.1986	-5.1986	-5.0328	-5.0328	-5.0328	-4.9927	-4.9927	-4.9927
10 000	-5.2596	-5.2597	-5.2596	-5.1006	-5.1006	-5.1006	-5.0679	-5.0679	-5.0679
11 000	-5.3558	-5.3558	-5.3558	-5.2029	-5.2030	-5.2029	-5.1765	-5.1765	-5.1765
12 000	-5.4131	-5.4132	-5.4131	-5.2607	-5.2607	-5.2607	-5.2352	-5.2352	-5.2352
13 000	-5.4534	-5.4534	-5.4534	-5.3007	-5.3007	-5.3007	-5.2753	-5.2754	-5.2753
14 000	-5.4876	-5.4877	-5.4876	-5.3348	-5.3349	-5.3348	-5.3091	-5.3091	-5.3091
15 000	-5.5202	-5.5203	-5.5202	-5.3675	-5.3675	-5.3675	-5.3399	-5.3399	-5.3399

TABLE XII.- ELECTRON NUMBER DENSITY N_e AT $p = 10p_o$

[0.1143^{12} means 0.1143×10^{12}, etc.]

T, °K	Electron number density for CO_2 determined by –			Electron number density for Mars atmosphere determined by –			Electron number density for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	-------	-------	-------	-------	-------	-------	-------	-------	-------
1 500	-------	-------	-------	-------	-------	-------	-------	-------	-------
2 000	-------	-------	-------	-------	-------	-------	-------	-------	-------
2 500	-------	-------	-------	-------	-------	-------	-------	-------	-------
3 000	-------	-------	-------	-------	-------	-------	-------	-------	-------
3 500	0.1143^{12}	0.1144^{12}	0.1138^{12}	0.2061^{13}	0.2061^{13}	0.2065^{13}	0.3110^{13}	0.3111^{13}	0.3125^{13}
4 000	$.1404^{13}$	$.1404^{13}$	$.1395^{13}$	$.1654^{14}$	$.1654^{14}$	$.1654^{14}$	[a]$.2432^{14}$	$.2432^{14}$	[a]$.2436^{14}$
4 500	$.8085^{13}$	$.8085^{13}$	$.7981^{13}$	$.7381^{14}$	$.7382^{14}$	$.7358^{14}$	$.1075^{15}$	$.1075^{15}$	$.1073^{15}$
5 000	$.2929^{14}$	$.2929^{14}$	$.2880^{14}$	$.2223^{15}$	$.2223^{15}$	$.2207^{15}$	$.3238^{15}$	$.3237^{15}$	$.3218^{15}$
5 500	$.9258^{14}$	$.9258^{14}$	$.9152^{14}$	$.5221^{15}$	$.5221^{15}$	$.5171^{15}$	$.7607^{15}$	$.7607^{15}$	$.7537^{15}$
6 000	$.2877^{15}$	$.2877^{15}$	$.2865^{15}$	$.1046^{16}$	$.1046^{16}$	$.1034^{16}$	$.1509^{16}$	$.1509^{16}$	$.1491^{16}$
6 500	$.8640^{15}$	$.8642^{15}$	$.8667^{15}$	$.1919^{16}$	$.1919^{16}$	$.1897^{16}$	[a]$.2637^{16}$	$.2637^{16}$	[a]$.2600^{16}$
7 000	$.2513^{16}$	$.2514^{16}$	$.2541^{16}$	$.3582^{16}$	$.3582^{16}$	$.3563^{16}$	$.4190^{16}$	$.4190^{16}$	$.4121^{16}$
7 500	$.6814^{16}$	$.6817^{16}$	$.6920^{16}$	$.7339^{16}$	$.7340^{16}$	$.7371^{16}$	$.6290^{16}$	$.6289^{16}$	$.6180^{16}$
8 000	$.1597^{17}$	$.1597^{17}$	$.1620^{17}$	$.1494^{17}$	$.1495^{17}$	$.1505^{17}$	$.9412^{16}$	$.9412^{16}$	$.9270^{16}$
8 500	$.3150^{17}$	$.3151^{17}$	$.3182^{17}$	$.2748^{17}$	$.2749^{17}$	$.2763^{17}$	$.1461^{17}$	$.1461^{17}$	$.1447^{17}$
9 000	$.5390^{17}$	$.5391^{17}$	$.5421^{17}$	$.4552^{17}$	$.4553^{17}$	$.4567^{17}$	$.2329^{17}$	$.2329^{17}$	$.2316^{17}$
9 500	$.8350^{17}$	$.8351^{17}$	$.8375^{17}$	$.6975^{17}$	$.6976^{17}$	$.6986^{17}$	$.3681^{17}$	$.3681^{17}$	$.3670^{17}$
10 000	$.1210^{18}$	$.1210^{18}$	$.1212^{18}$	$.1011^{18}$	$.1011^{18}$	$.1012^{18}$	$.5648^{17}$	$.5648^{17}$	$.5639^{17}$
11 000	$.2224^{18}$	$.2224^{18}$	$.2225^{18}$	$.1891^{18}$	$.1891^{18}$	$.1891^{18}$	$.1196^{18}$	$.1196^{18}$	$.1195^{18}$
12 000	$.3601^{18}$	$.3602^{18}$	$.3602^{18}$	$.3148^{18}$	$.3149^{18}$	$.3148^{18}$	$.2221^{18}$	$.2221^{18}$	$.2220^{18}$
13 000	$.5290^{18}$	$.5291^{18}$	$.5290^{18}$	$.4785^{18}$	$.4786^{18}$	$.4785^{18}$	$.3693^{18}$	$.3693^{18}$	$.3693^{18}$
14 000	$.7174^{18}$	$.7175^{18}$	$.7174^{18}$	$.6737^{18}$	$.6737^{18}$	$.6736^{18}$	$.5584^{18}$	$.5585^{18}$	$.5584^{18}$
15 000	$.9108^{18}$	$.9109^{18}$	$.9108^{18}$	$.8861^{18}$	$.8862^{18}$	$.8861^{18}$	$.7763^{18}$	$.7764^{18}$	$.7763^{18}$

[a] Recomputed value (see text).

TABLE XIII.- ELECTRON NUMBER DENSITY N_e AT $p = 10^{-3}p_o$

[0.1871^{9} means 0.1871×10^{9}, etc.]

T, °K	Electron number density for CO_2 determined by –			Electron number density for Mars atmosphere determined by –			Electron number density for air determined by –		
	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator	Direct summation	Modified method	Rotating harmonic oscillator
1 000	-------	-------	-------	-------	-------	-------	-------	-------	-------
1 500	-------	-------	-------	-------	-------	-------	-------	-------	-------
2 000	-------	-------	-------	-------	-------	-------	-------	-------	-------
2 500	-------	- -------	-------	-------	-------	-------	-------	-------	-------
3 000	-------	-------	-------	-------	-------	-------	-------	-------	-------
3 500	0.1871^{9}	0.1871^{9}	0.1862^{9}	0.5537^{10}	0.5537^{10}	0.5502^{10}	0.8226^{10}	0.8226^{10}	0.8174^{10}
4 000	$.3139^{10}$	$.3139^{10}$	$.3143^{10}$	$.2654^{11}$	$.2655^{11}$	$.2634^{11}$	$.3932^{11}$	$.3933^{11}$	$.3901^{11}$
4 500	$.5306^{11}$	$.5307^{11}$	$.5371^{11}$	[a]$.9651^{11}$	$.9650^{11}$	[a]$.9611^{11}$	$.1231^{12}$	$.1232^{12}$	$.1219^{12}$
5 000	$.7594^{12}$	$.7595^{12}$	$.7698^{12}$	$.7113^{12}$	$.7114^{12}$	$.7186^{12}$	$.2730^{12}$	$.2731^{12}$	$.2695^{12}$
5 500	$.4506^{13}$	$.4507^{13}$	$.4530^{13}$	$.3677^{13}$	$.3677^{13}$	$.3691^{13}$	$.6606^{12}$	$.6603^{12}$	$.6569^{12}$
6 000	$.1377^{14}$	$.1377^{14}$	$.1378^{14}$	$.1085^{14}$	$.1085^{14}$	$.1086^{14}$	$.2048^{13}$	$.2047^{13}$	$.2046^{13}$
6 500	$.3186^{14}$	$.3186^{14}$	$.3187^{14}$	$.2492^{14}$	$.2493^{14}$	$.2493^{14}$	$.5887^{13}$	$.5888^{13}$	$.5886^{13}$
7 000	$.6211^{14}$	$.6212^{14}$	$.6212^{14}$	$.4838^{14}$	$.4839^{14}$	$.4839^{14}$	$.1470^{14}$	$.1470^{14}$	$.1470^{14}$
7 500	$.1039^{15}$	$.1039^{15}$	$.1039^{15}$	$.8074^{14}$	$.8075^{14}$	$.8074^{14}$	$.3222^{14}$	$.3222^{14}$	$.3221^{14}$
8 000	$.1500^{15}$	$.1500^{15}$	$.1500^{15}$	$.1179^{15}$	$.1179^{15}$	$.1179^{15}$	$.6268^{14}$	$.6269^{14}$	$.6268^{14}$
8 500	$.1916^{15}$	$.1916^{15}$	$.1916^{15}$	$.1575^{15}$	$.1575^{15}$	$.1575^{15}$	$.1087^{15}$	$.1087^{15}$	$.1087^{15}$
9 000	$.2281^{15}$	$.2282^{15}$	$.2281^{15}$	$.2014^{15}$	$.2014^{15}$	$.2014^{15}$	$.1676^{15}$	$.1676^{15}$	$.1676^{15}$
9 500	$.2623^{15}$	$.2623^{15}$	$.2623^{15}$	$.2468^{15}$	$.2469^{15}$	$.2468^{15}$	$.2285^{15}$	$.2285^{15}$	$.2285^{15}$
10 000	$.2906^{15}$	$.2907^{15}$	$.2906^{15}$	$.2842^{15}$	$.2843^{15}$	$.2842^{15}$	$.2764^{15}$	$.2764^{15}$	$.2764^{15}$
11 000	$.3119^{15}$	$.3120^{15}$	$.3119^{15}$	$.3119^{15}$	$.3120^{15}$	$.3119^{15}$	$.3109^{15}$	$.3109^{15}$	$.3109^{15}$
12 000	$.3003^{15}$	$.3003^{15}$	$.3003^{15}$	$.3005^{15}$	$.3006^{15}$	$.3005^{15}$	$.3004^{15}$	$.3004^{15}$	$.3004^{15}$
13 000	$.2808^{15}$	$.2808^{15}$	$.2808^{15}$	$.2809^{15}$	$.2809^{15}$	$.2809^{15}$	$.2808^{15}$	$.2808^{15}$	$.2808^{15}$
14 000	$.2620^{15}$	$.2620^{15}$	$.2620^{15}$	$.2620^{15}$	$.2620^{15}$	$.2620^{15}$	$.2617^{15}$	$.2617^{15}$	$.2617^{15}$
15 000	$.2460^{15}$	$.2460^{15}$	$.2460^{15}$	$.2460^{15}$	$.2461^{15}$	$.2460^{15}$	$.2447^{15}$	$.2447^{15}$	$.2447^{15}$

[a] Recomputed value (see text).

TABLE XIV.- RECIPROCAL MOLECULAR WEIGHT RATIO 1/Z COMPARISONS FOR AIR

T, °K	Reciprocal molecular weight ratio determined by – Modified method	Browne, reference 8	Gilmore, references 1 and 5
	$\log_{10} \frac{\rho}{\rho_0} = 0.000$		
1 000	0.99999	------	1.0000
2 000	.99994	------	1.0000
3 000	.99280	0.99285	.9929
4 000	.94068	.94082	.9409
5 000	.87337	.87329	.8735
6 000	.83443	.83452	.8344
7 000	.78713	.78715	.7875
8 000	.71435	.71423	.7142
10 000	.56905	.56857	.5688
12 000	.51112	.51041	.5110
15 000	.47765	.47765	------
18 000	.43756	.43771	.4378
21 000	.39116	.39151	------
24 000	.35008	.35078	.3490
	$\log_{10} \frac{\rho}{\rho_0} = -3.000$		
1 000	0.99999	------	1.0000
2 000	.99823	------	.9983
3 000	.88159	0.88168	.8818
4 000	.82595	.82604	.8260
5 000	.76420	.76418	.7645
6 000	.60076	.60067	.6009
7 000	.51580	.51578	.5159
8 000	.49956	.49960	.4998
10 000	.46274	.46292	.4634
12 000	.37815	.37847	.3794
15 000	.27861	.27872	-----
18 000	.25576	.25578	.2558
21 000	.25097	.25098	-----
24 000	.24168	.24170	.2414

TABLE XV.- NONDIMENSIONAL ENTHALPY H/ZRT COMPARISONS FOR AIR

T, °K	Nondimensional enthalpy determined by – Modified method	Browne, reference 8	Gilmore, references 1 and 5
	$\log_{10} \frac{\rho}{\rho_0} = 0.000$		
1 000	3.6305	-----	3.630
2 000	3.9604	-----	3.962
3 000	4.3702	4.3724	4.371
4 000	5.0873	5.0867	5.088
5 000	5.4896	5.4898	5.488
6 000	5.5953	5.5932	5.591
7 000	5.9352	5.9335	5.932
8 000	6.5351	6.5342	6.531
10 000	7.3611	7.3650	[a]7.490
12 000	7.2188	7.2254	7.224
15 000	6.8391	6.8410	----
18 000	6.7478	6.7568	6.709
21 000	6.7565	6.7790	----
24 000	6.6931	6.7261	6.616
	$\log_{10} \frac{\rho}{\rho_0} = -3.000$		
1 000	3.6305	-----	3.630
2 000	4.0058	-----	4.007
3 000	6.1284	6.1273	6.127
4 000	6.2603	6.2592	6.263
5 000	7.0640	7.0629	7.061
6 000	9.3453	9.3458	9.346
7 000	9.7384	9.7384	9.744
8 000	9.1929	9.1922	9.196
10 000	8.8180	8.8147	8.813
12 000	9.4072	9.4036	9.399
15 000	9.4986	9.5006	----
18 000	8.6410	8.6439	8.650
21 000	7.8908	7.8932	----
24 000	7.5887	7.5901	7.609

[a] Gilmore (ref. 5) notes that this value disagrees with the value 7.380 from reference 2.

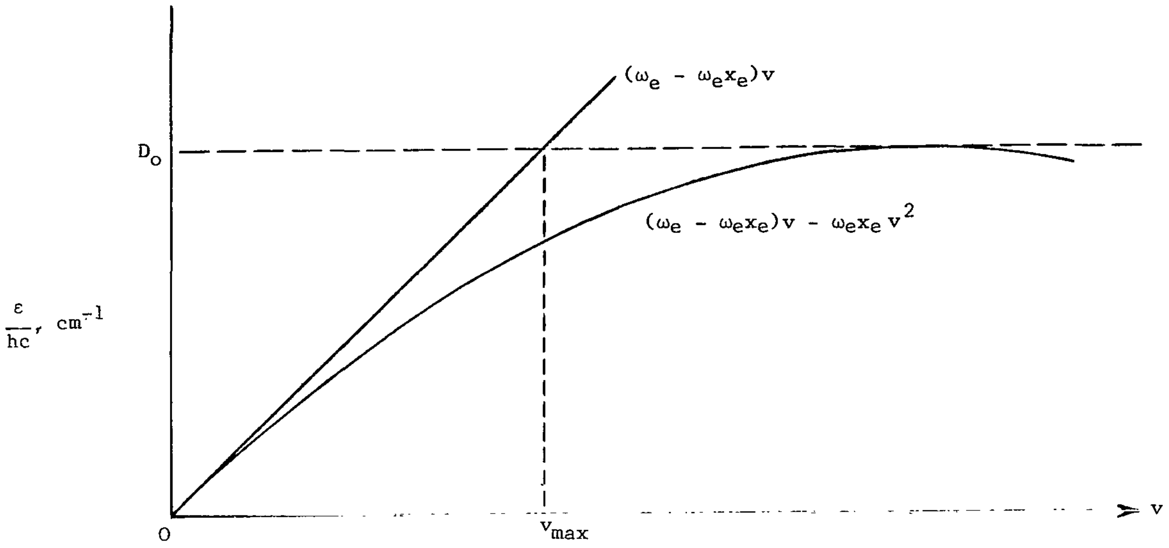
TABLE XVI.- NONDIMENSIONAL ENTROPY S/R COMPARISONS FOR AIR

T, °K	Nondimensional entropy determined by –		
	Modified method	Browne, reference 8	Gilmore, references 1 and 5
	$\log_{10} \frac{\rho}{\rho_o} = 0.000$		
1 000	27.034	-----	26.83
2 000	29.290	-----	29.29
3 000	30.997	31.000	30.98
4 000	33.042	33.042	33.03
5 000	34.906	34.906	34.91
6 000	36.242	36.238	36.25
7 000	37.903	37.898	37.88
8 000	40.308	40.305	40.32
10 000	45.857	45.872	45.74
12 000	49.005	49.034	49.00
15 000	51.781	51.783	----
18 000	54.987	55.003	54.88
21 000	58.708	58.755	----
24 000	62.327	62.396	62.09
	$\log_{10} \frac{\rho}{\rho_o} = -3.000$		
1 000	33.942	-----	33.74
2 000	36.253	-----	36.26
3 000	40.668	40.666	40.65
4 000	43.043	43.041	43.05
5 000	46.127	46.125	46.11
6 000	54.013	54.016	54.00
7 000	59.519	59.519	59.51
8 000	61.213	61.209	61.20
10 000	65.341	65.324	65.30
12 000	74.164	74.128	74.03
15 000	88.438	88.422	----
18 000	93.398	93.398	93.38
21 000	95.394	95.395	----
24 000	98.811	98.809	98.93

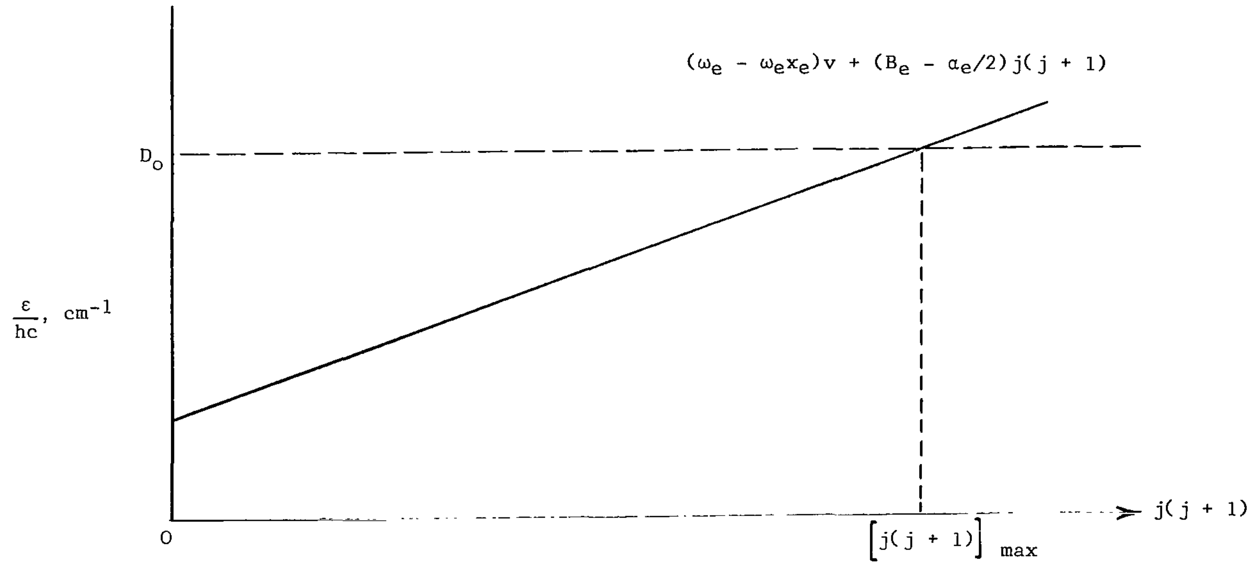
TABLE XVII.- ELECTRON NUMBER DENSITY N_e COMPARISONS FOR AIR

[0.1822^{12} means 0.1822×10^{12}, etc.]

T, °K	Electron number density determined by –		
	Modified method	Browne, reference 8	Gilmore, references 1 and 5
	$\log_{10} \frac{\rho}{\rho_o} = 0.000$		
1 000	-------	-------	------
2 000	-------	-------	------
3 000	0.1822^{12}	0.1802^{12}	0.195^{12}
4 000	$.3043^{14}$	$.3038^{14}$	$.328^{14}$
5 000	$.5226^{15}$	$.5216^{15}$	$.562^{15}$
6 000	$.3017^{16}$	$.3011^{16}$	$.324^{16}$
7 000	$.1024^{17}$	$.1021^{17}$	$.109^{17}$
8 000	$.2657^{17}$	$.2645^{17}$	$.280^{17}$
10 000	$.1538^{18}$	$.1532^{18}$	$.154^{18}$
12 000	$.6746^{18}$	$.6727^{18}$	$.669^{18}$
15 000	$.3022^{19}$	$.3015^{19}$	------
18 000	$.7989^{19}$	$.7971^{19}$	$.795^{19}$
21 000	$.1522^{20}$	$.1518^{20}$	------
24 000	$.2324^{20}$	$.2313^{20}$	$.235^{20}$
	$\log_{10} \frac{\rho}{\rho_o} = -3.000$		
1 000	-------	-------	------
2 000	-------	-------	------
3 000	0.5592^{10}	0.5571^{10}	0.605^{10}
4 000	$.3432^{12}$	$.3424^{12}$	$.369^{12}$
5 000	$.3680^{13}$	$.3672^{13}$	$.396^{13}$
6 000	$.1899^{14}$	$.1893^{14}$	$.198^{14}$
7 000	$.1087^{15}$	$.1080^{15}$	$.108^{15}$
8 000	$.5141^{15}$	$.5110^{15}$	$.503^{15}$
10 000	$.4582^{16}$	$.4562^{16}$	$.451^{16}$
12 000	$.1756^{17}$	$.1751^{17}$	$.173^{17}$
15 000	$.4295^{17}$	$.4294^{17}$	------
18 000	$.5159^{17}$	$.5159^{17}$	$.516^{17}$
21 000	$.5360^{17}$	$.5360^{17}$	------
24 000	$.5771^{17}$	$.5771^{17}$	$.579^{17}$



(a) Maximum v from the j = 0 case, v_{max}.



(b) Maximum j for a given v, $j(v)_{max}$.

Figure 1.- Method for determining approximate v_{max} and $j(v)_{max}$ for an excited electronic state of a diatomic species.

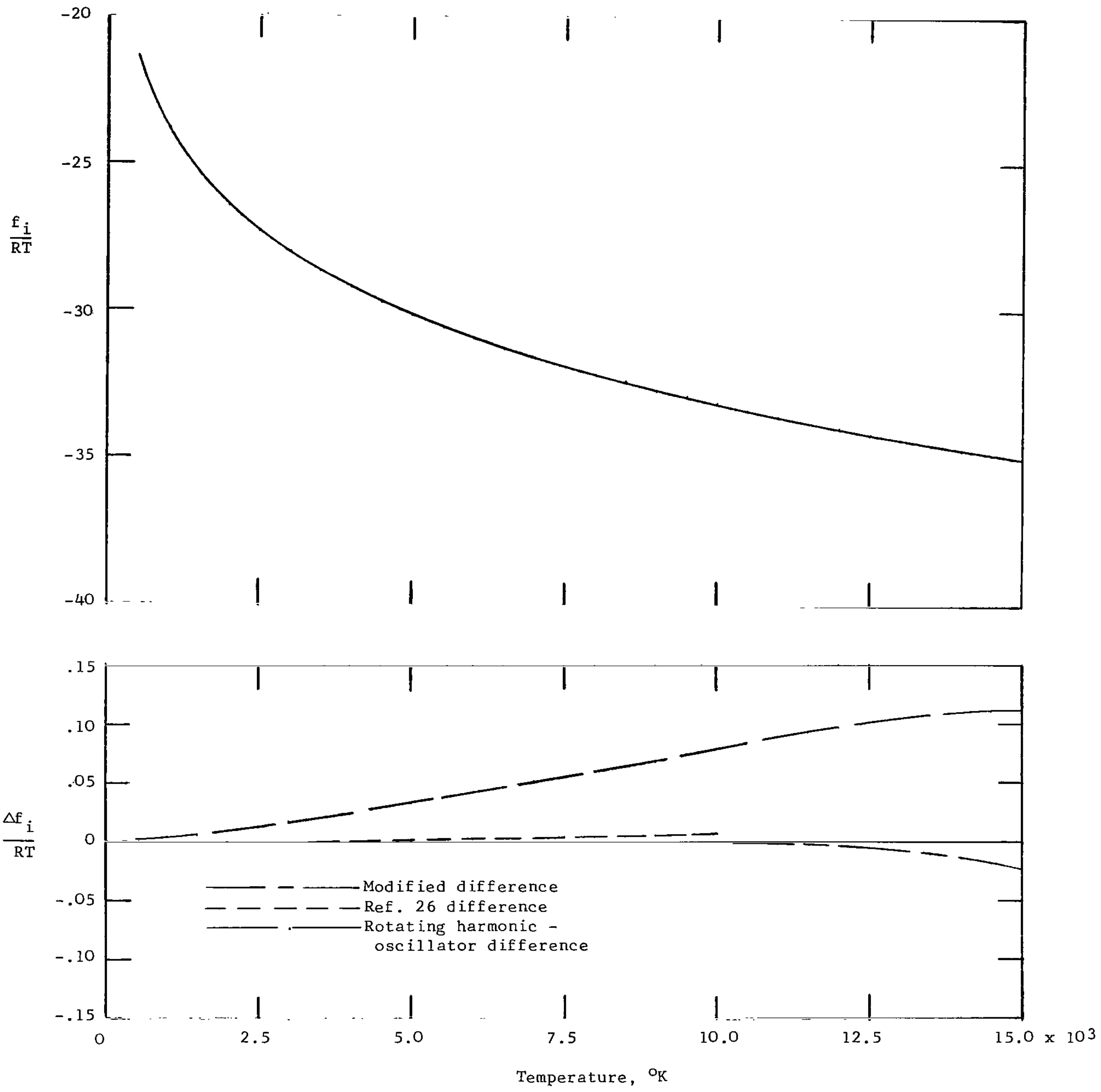


Figure 2.- Variation with temperature of Gibbs free energy of N_2 at $p = p_0$ determined by the direct-summation method and the differences between results from the direct summation and other methods. Note that the difference scale is magnified.

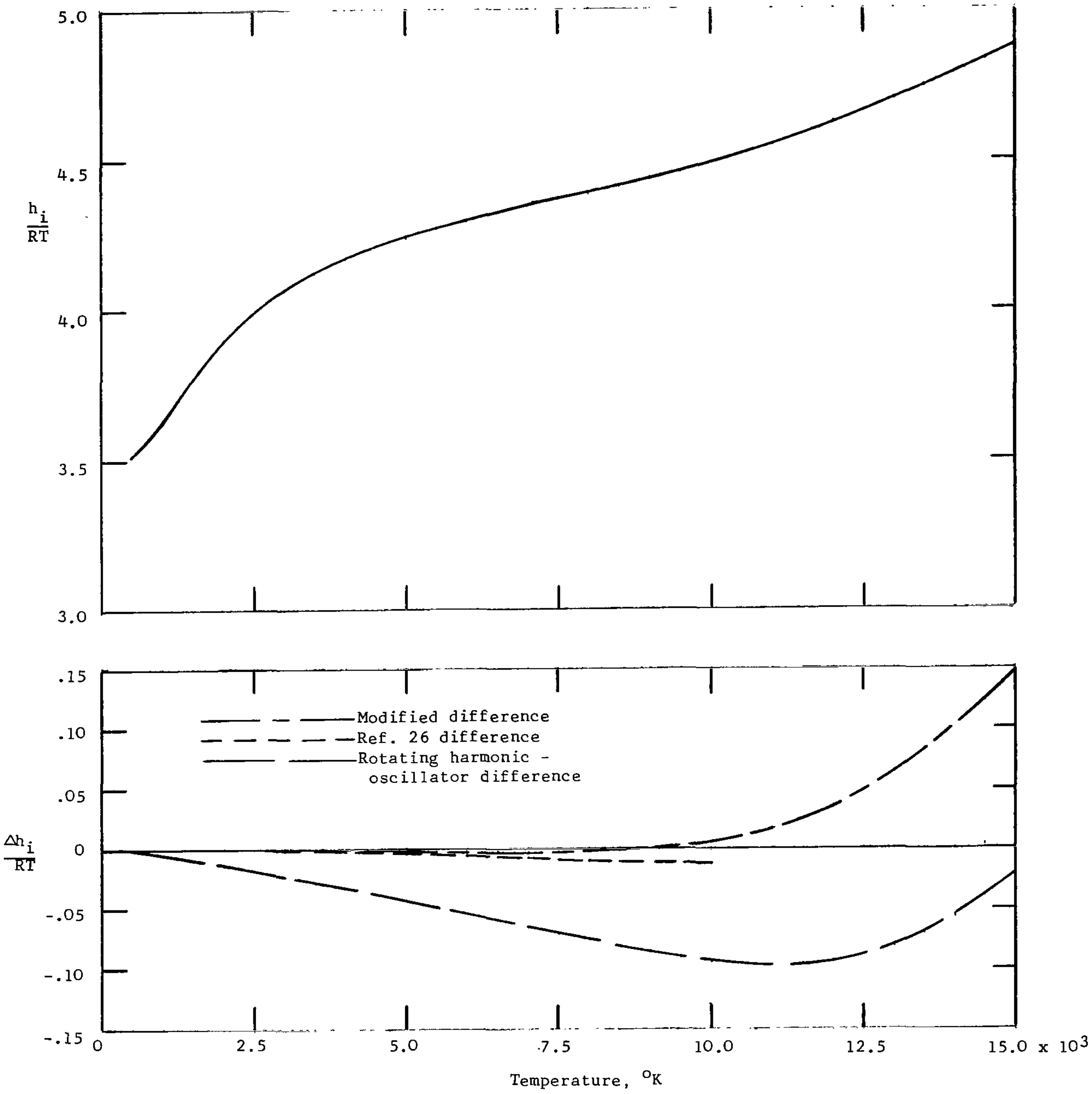


Figure 3.- Variation with temperature of enthalpy of N_2 at $p = p_0$ determined by the direct-summation method and the differences between results from the direct summation and other methods. Note that the difference scale is magnified.

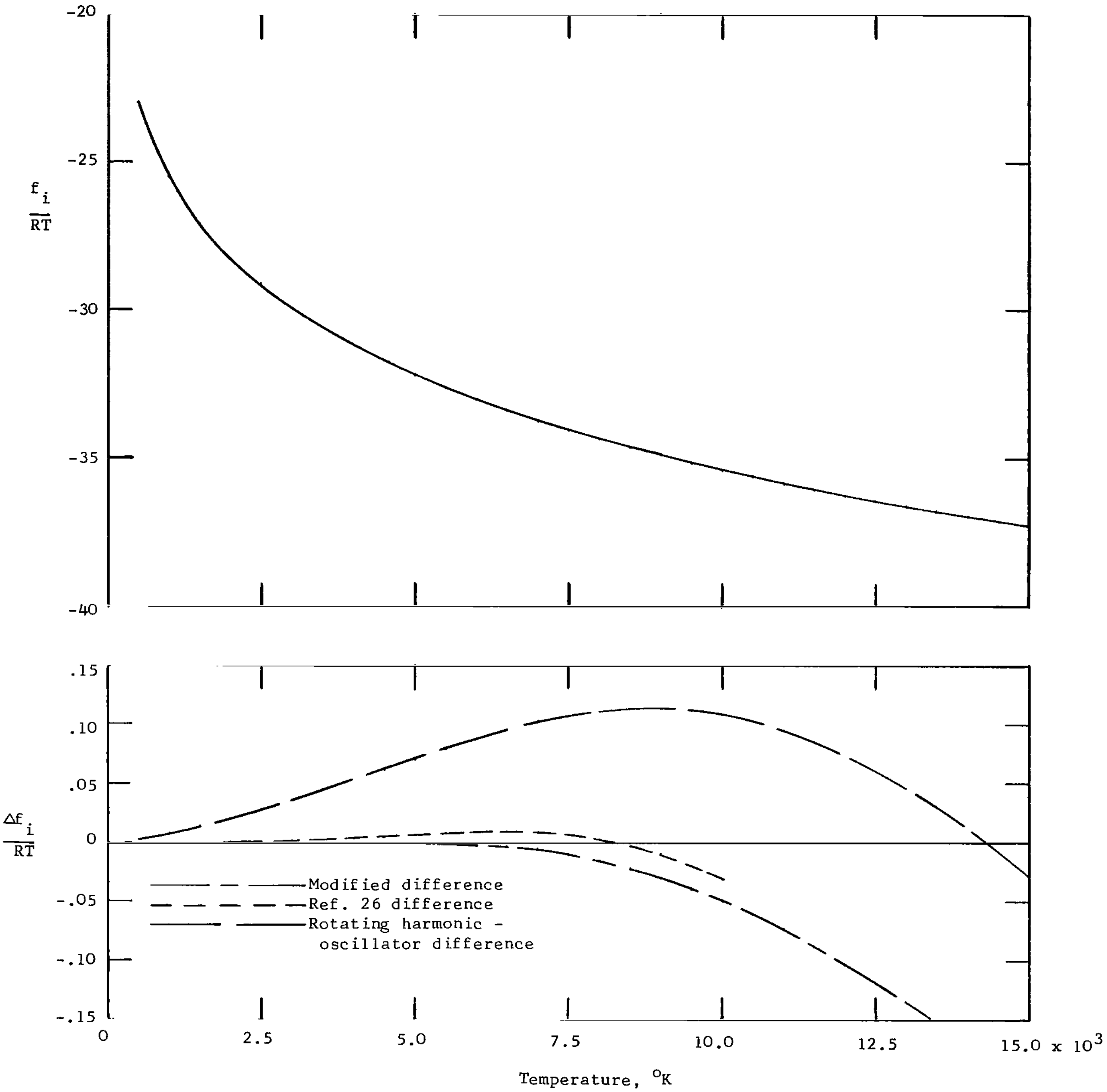


Figure 4.- Variation with temperature of Gibbs free energy of O_2 at $p = p_0$ determined by the direct-summation method and the differences between results from the direct summation and other methods. Note that the difference scale is magnified.

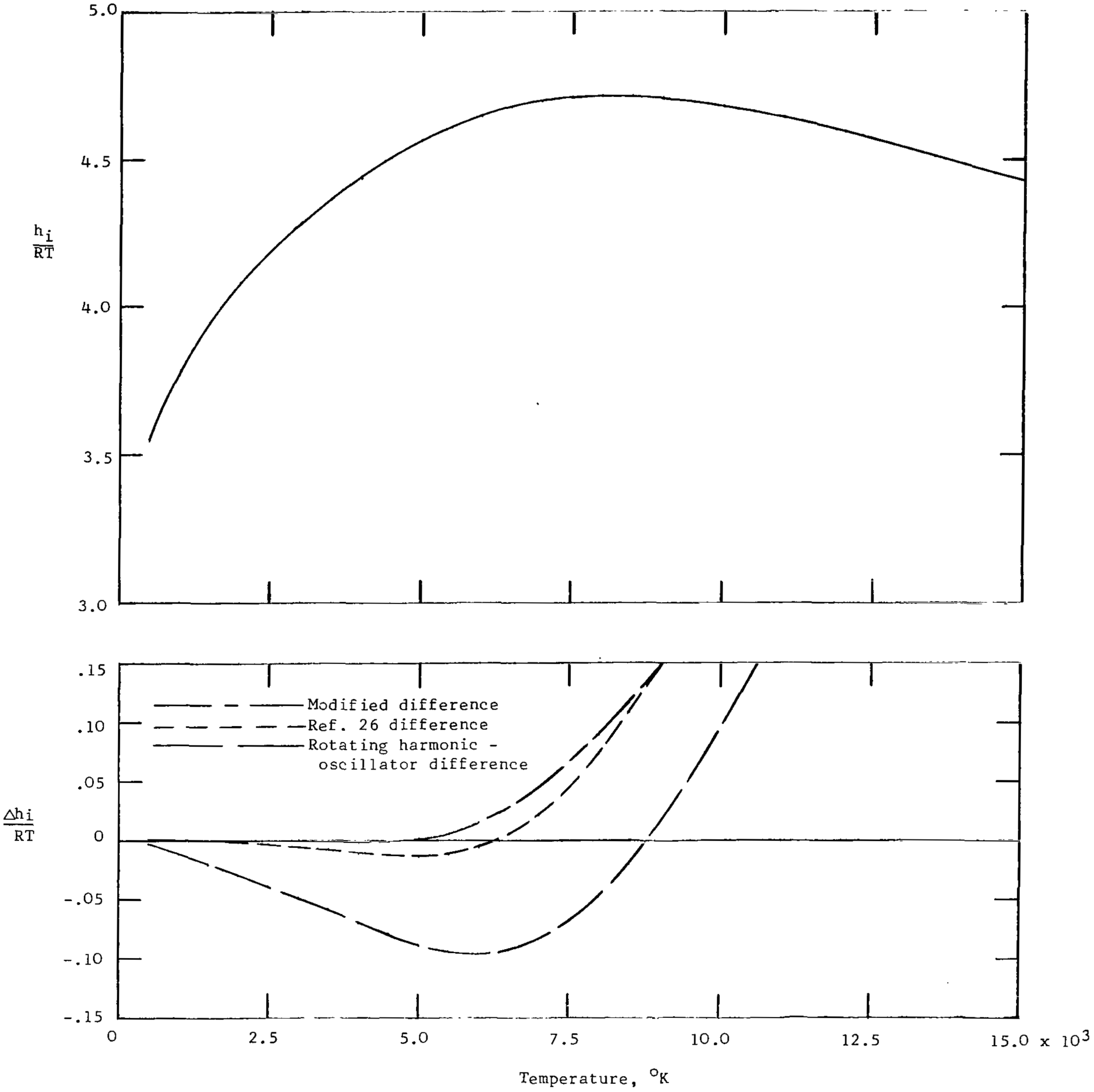
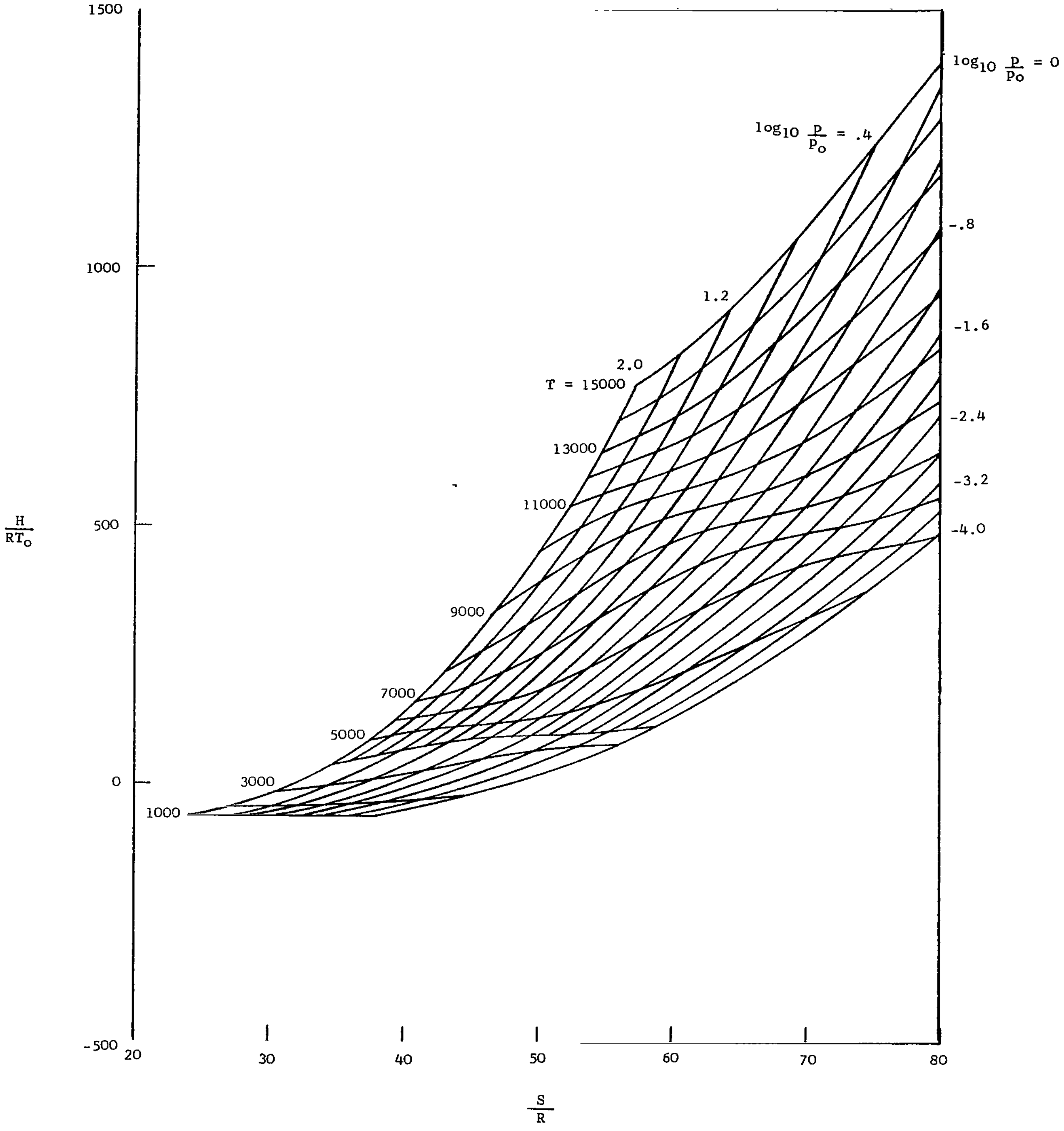
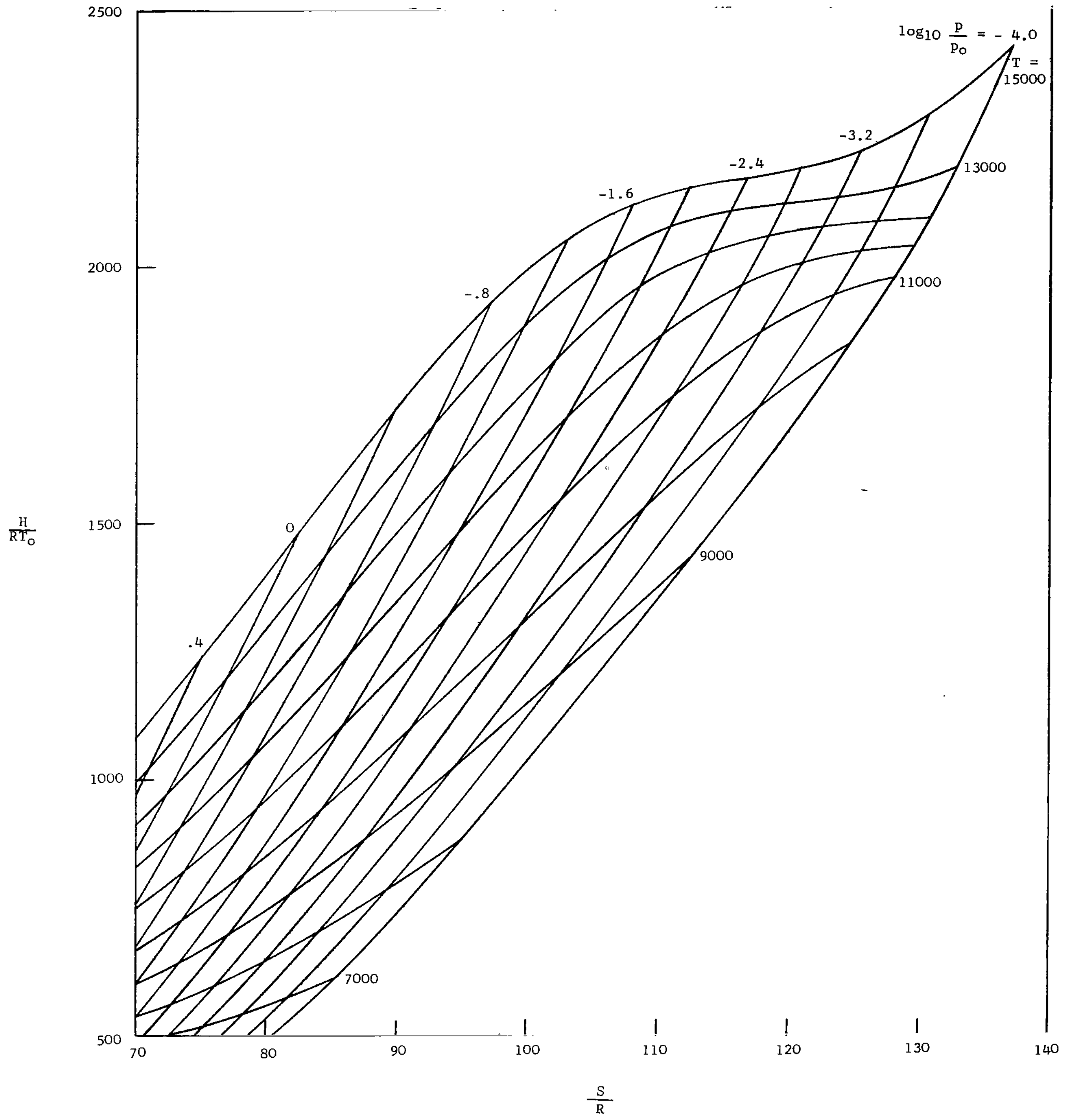


Figure 5.- Variation with temperature of enthalpy of O_2 at $p = p_0$ determined by the direct-summation method and the differences between results from the direct summation and other methods. Note that the difference scale is magnified.



(a) $\frac{H}{RT_0} = -500$ to 1500.

Figure 6.- Mollier diagram for "Mars" atmosphere; 25 percent N_2, 32 percent Ar, and 43 percent CO_2 by volume.



(b) $\frac{H}{RT_0}$ = 500 to 2500.

Figure 6.- Concluded.

NASA-Langley, 1966 L-4547

> *"The aeronautical and space activities of the United States shall be conducted so as to contribute . . . to the expansion of human knowledge of phenomena in the atmosphere and space. The Administration shall provide for the widest practicable and appropriate dissemination of information concerning its activities and the results thereof."*
>
> —NATIONAL AERONAUTICS AND SPACE ACT OF 1958

NASA SCIENTIFIC AND TECHNICAL PUBLICATIONS

TECHNICAL REPORTS: Scientific and technical information considered important, complete, and a lasting contribution to existing knowledge.

TECHNICAL NOTES: Information less broad in scope but nevertheless of importance as a contribution to existing knowledge.

TECHNICAL MEMORANDUMS: Information receiving limited distribution because of preliminary data, security classification, or other reasons.

CONTRACTOR REPORTS: Technical information generated in connection with a NASA contract or grant and released under NASA auspices.

TECHNICAL TRANSLATIONS: Information published in a foreign language considered to merit NASA distribution in English.

TECHNICAL REPRINTS: Information derived from NASA activities and initially published in the form of journal articles.

SPECIAL PUBLICATIONS: Information derived from or of value to NASA activities but not necessarily reporting the results of individual NASA-programmed scientific efforts. Publications include conference proceedings, monographs, data compilations, handbooks, sourcebooks, and special bibliographies.

Details on the availability of these publications may be obtained from:

SCIENTIFIC AND TECHNICAL INFORMATION DIVISION
NATIONAL AERONAUTICS AND SPACE ADMINISTRATION
Washington, D.C. 20546