

A SET OF PARTITION FUNCTIONS AND EQUILIBRIUM CONSTANTS FOR 300 DIATOMIC MOLECULES OF ASTROPHYSICAL INTEREST

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ABSTRACT

Polynomial developments for partition functions and equilibrium constants of 300 diatomic molecules and of relevant atoms are given for a temperature range from 1000 to 9000 K. All molecular spectroscopic data, with a few exceptions, are derived from the book by Huber and Herzberg in order to lead to a homogeneous set of data.

Subject heading: molecular processes

I. INTRODUCTION

Important progress has been made in recent years in the interpretation of molecular bands in stellar and cometary spectra. High-resolution spectrophotometric tracings have been obtained in the infrared as well as in the visible and ultraviolet regions, representative model atmospheres have been computed, and computer programs for the generation of synthetic spectra have been developed.

Of fundamental importance in the interpretation of molecular bands in astrophysical sources has been the calculation of the relative abundances of different molecules in a stellar atmosphere as a function of temperature, pressure, and initial elemental composition. The pioneering paper of this nature was that of Russell (1934). In the last 25 years, with the development of computers and with better knowledge of molecular constants, calculations of this type have been performed by many authors. We may cite the paper of Tsuji (1964) as being representative of one of the more extensive of these calculations from the modern era. The results of the calculations to which we refer are usually presented as graphs in which the predicted abundances of various molecular species are displayed as a function of temperature. Any comparison of the results of the calculations by different authors quickly reveals numerous differences, some minor, some major. It is rarely clear whether such differences are of astrophysical significance, reflecting differences in the stellar atmospheric model, the pressure, or the elemental composition, or whether such differences are mere artifacts of the calculations resulting from different assumed values of molecular parameters such as partition functions and equilibrium constants. In some cases apparent large differences in deduced elemental abundances can be shown to vanish if the same initial molecular constants are used in different calculations. Of particular importance in the equilibrium constant is the dissociation energy D_0^0 . The assumed value of D_0^0 should always be quoted in such calculations. For example, our knowledge of the dissociation energy of monoxides such as TiO and ZrO has changed over the years. Further, large differences in partition functions of these same molecules arise from the inclusion of low-lying states of high multiplicity.

It is our strong suggestion, therefore, that if meaningful comparisons between abundance determinations are to be made and meaningful astrophysical conclusions are to be drawn from calculations on different atmospheric models, it is highly desirable or essential that all such calculations be based on a standard set of molecular partition functions and equilibrium constants. It is, in our view, more important for calculations to be based on a single, unified, coherent body of molecular data than for workers to attempt to keep up with every minor improvement in rotational and vibrational constants that appears month by month in the molecular literature. Only in cases where a dissociation energy is shown to be grossly wrong or where undiscovered low-lying states later discovered would it be important to depart from the standard set of equilibrium constants.

Fortunately, a large coherent and critical body of molecular constants has in recent years become available in the compilation of Huber and Herzberg (1979), and we have preferred to adopt the data in that unique compilation to compute what we hope will be a standard set of molecular partition functions and dissociation equilibrium constants. We do not assert that there are no errors in Huber and Herzberg's book, nor that improvements to the molecular constants therein will never be made. The essential point, however, is that there can be no ambiguity about what values of the molecular constants were used in our calculations of partition functions and equilibrium constants. For this reason we have deliberately avoided critical discussion about the published constants. If calculations of molecular equilibria were to be made using this same set of standard constants, then any differences that appear will be of astronomical significance, unhidden by minor variations in assumed molecular data.

There are important uses for both partition functions (excitation processes) and equilibrium constants (dissociation processes) in astrophysical work, and we have therefore elected to calculate and tabulate both. Rather than tabulate these quantities as functions

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$T \approx 10-1000\text{ K}$.

P

$$10^{-9} \text{ g/cm}^3$$

10^{-42}

11

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194 of temperature for small temperature intervals over a wide temperature range, such as in the JANAF tables (Stull and Prophet 1971; Chase *et al.* 1974, 1975, 1978), it is more useful to give polynomial expansions as functions of temperature. Not only does this take up far less space, but it is much more readily adaptable to computer calculations.

The temperature range we have chosen is 1000–9000 K. Few molecules survive in stellar atmospheres above 9000 K. Below 1000 K molecules appear in such astronomical sources as comets and interstellar gas clouds. At such temperatures, a well-known approximation to the rotational partition function breaks down. More important, such sources are usually far from thermodynamic equilibrium, and it would be misleading to think that the elementary theory of molecular dissociation equilibrium is valid in such sources. For these reasons our calculations are restricted to temperatures between 1000 and 9000 K.

We deal with 300 diatomic molecules of known or possible astrophysical interest for which molecular data are given in Huber and Herzberg. Always during preparation of this paper we have been aware of revised molecular constants appearing in the literature. For example, Colket (1984) has found $D_0^0 = 7.95$ eV for CN. However, the need for homogeneity and certainty as to which data we have used has overridden relatively minor corrections, and we have retained Huber and Herzberg's values. The only exception for which we felt it was important to depart from this policy was to recognize the placement of the $a^3\Delta$ state (and consequently all other triplet states) of ZrO by Phillips and Davis (1979). There are known to be other molecules of importance in astronomy for which molecular constants have not yet been measured. For these it may be possible to give a reasonably reliable estimate of partition functions and equilibrium constants. This will be the subject of a later paper by A. J. S. and R. Heffnerlin based on a search for periodicities in the partition functions of selected molecular species (isoelectronic compounds, etc.)

II. POLYNOMIAL EXPANSIONS FOR PARTITION FUNCTIONS

Following the early work of Gibson and Heitler (1928), many papers have been devoted to the exact calculation of all quantities entering the expressions for the partition function and equilibrium constant. Very elaborate expressions can be derived to calculate exactly the partition function as a function of temperature. For the temperature range of interest, equation (15) of Tatum (1966) is probably adequate. The adopted molecular model abandons the Born-Oppenheimer approximation: it includes higher electronic states, electronic-vibrational-rotational interaction, and anharmonicity, but it retains the high-temperature approximation to the rotational partition function mentioned earlier:

$$Q = \exp \left[\frac{hc}{kT} \left(\frac{1}{2} \omega_{e_1} - \frac{1}{4} \omega_{e_1} x_{e_1} \right) \right] \sum_e^{40000 \text{ cm}^{-1}} \sum_{v=0}^{u_{\max}} \frac{g_e k T}{\sigma h c} \left[B_e - \alpha_e \left(v + \frac{1}{2} \right) \right]^{-1} \\ \times \exp \left\{ -\frac{hc}{kT} \left[\omega_e \left(v + \frac{1}{2} \right) - \omega_e x_e \left(v + \frac{1}{2} \right)^2 + T_e \right] \right\}. \quad (1)$$

We must note that higher order correction constants are seldom known for the selected molecules. Moreover, even first-order terms (α_e , $\omega_e x_e$) are still lacking for some of them. While exact formulas, including high-order constants, are essential for generating precise wavenumbers, their effect on calculations of thermodynamic functions is small and unlikely to be of significance in any astrophysical context. In any case, some authors have made a detailed comparison between different approximations generally proposed in the past, using specific relations or expansions (see, e.g., Witschel 1974). The direct summation, which leads to the exact result, appears to differ rather little from approximations, such as for CO.

exact result, appears to differ rather little from approximations, such as for CO. Therefore, in order to get a homogeneous set of Q -values, we preferred to adopt the same simplified equation (1) for all molecules considered here. Moreover, the error in Q due to the adopted model remains always less than other sources of uncertainties (D^0 unobserved states, g , T_c , etc).

It is interesting to consider an example to investigate how Q , the partition function, varies with temperature, for example, in the case of H_2 with one electronic state. Figure 1 shows the variation of $\log Q$ with $\log T$. At low temperatures Q is almost independent of T ; at intermediate temperatures Q is approximately proportional to T ; and at higher temperatures Q is approximately proportional to T^2 .

We can compare this behavior, deduced from an exact calculation, with various approximations that have been used in different temperature ranges. Table 1 gives approximations for Q_{rot} and Q_{vib} in different regions. The asymptotic expression for Q_{rot} is classical, whereas the expression for Q_{vib} is derived from the approximation that, provided that $0 < x < 1.2$, where $x = hc\omega_e/kT$, the expression $(1 - e^{-x})/(xe^{-0.46x})$ is within 1% of unity, as explained by Russell (1934). Except for H₂ and some light hydrides, the expression $T^2 \exp(+0.66\omega_e/T)$ is approximately equal to T^2 , so that this asymptotic expression agrees approximately with the results of detailed calculations: namely, that for the higher temperatures, Q varies approximately as T^2 . Figure 2, relative to CO, illustrates this well and also shows the temperature variation of the equilibrium constant. This suggests that in the temperature range $T > 1000$ K, $\ln Q \approx \ln k + \ln T - \ln \log \theta$, where $\theta = 5040/T$.

For $T \geq 1.2 \omega_e$, more exact expressions for the partition function of a rotating harmonic oscillator with one electronic state are

$$\log Q = \log \frac{g_e}{\sigma R \omega} - 0.32 + 2 \log T + \frac{0.29 \omega_e}{T}, \quad (2)$$

DIATOMIC MOLECULE PARTITION FUNCTIONS

TABLE I
APPROXIMATE FORMULAE FOR Q_{rot} AND Q_{vib} IN DIFFERENT TEMPERATURE RANGES

Temperature Range ^a	Q_{rot}	Temperature Range ^b	Q_{vib}
Below $0.5B$	1	below $0.3\omega_e$	1
$0.5B - 3.7B$	J summation	$0.3\omega_e - 1.2\omega_e$	v summation
Above $3.7B$	$\frac{kT}{hcB} + \frac{1}{3}$	above $1.2\omega_e$	$\frac{kT}{hc\omega_e} \times 10^{0.29\omega_e/T}$

^a B is the rotational constant in cm^{-1} .
^b ω_e is the vibrational constant in cm^{-1} .

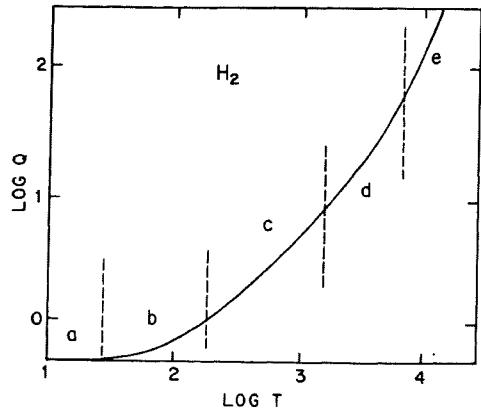


FIG. 1.

FIG. 1.—Partition function for H_2 . (a) $T < B/2$: Q_{rot} is almost independent of T and tends to $1/\sigma = \frac{1}{2}$ at very low temperature. (b) $B/2 \leq T \leq 3.7B$: Q_{rot} is best calculated by direct summation over J levels. (c) $3.7B < T$, and $T < 0.3\omega_e$: Q_{rot} is approximately linearly proportional to T . (d) $0.3 \leq T/\omega_e \leq 1.2$: Q_{vib} is best calculated by direct summation over v levels. (e) $1.2\omega_e < T$: $Q \propto T^2 e^{0.29\omega_e/T}$. T is the temperature in kelvins, and B and ω_e are the rotational and vibrational constants in inverse centimeters.

FIG. 2.—Partition function and equilibrium constant for CO

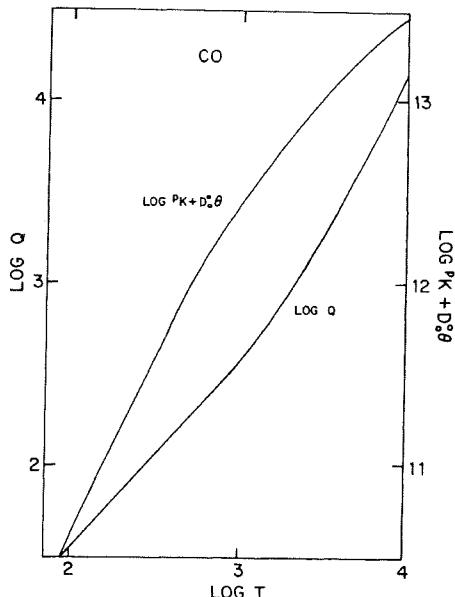


FIG. 2

or

$$\log Q = \log \frac{g_e}{\sigma B_e \omega_e} + 7.08 - 2 \log \theta + \frac{\omega_e \theta}{17,500}. \quad (3)$$

Here B_e and ω_e are the rotational and vibrational constants expressed in inverse centimeters, g_e is the multiplicity of the ground electronic state $(2 - \delta_{0,\Lambda})(2S + 1)$, and σ is the symmetry factor (1 for the heteronuclear molecule, 2 for a homonuclear molecule). We have preferred the second relation because in the temperature range of interest $|\log \theta| < 1$, which is a necessary condition for convergence.

In the past, several polynomial approximations for molecular partition functions have appeared in the literature, each with its own advantages and disadvantages. We show in Table 2 the expansions in the case of CO and offer some comments.

In Gurvich *et al.* (1962), the numerical coefficients correspond to the Gibbs energy function ϕ_T , which is related to the partition function by

$$\log Q(T) = 0.21855\phi_T - 2.5 \log T - 1.5 \log M + 1.5917, \quad (4)$$

where M is the mass of the molecule in atomic mass units and ϕ_T is in $\text{cal mol}^{-1} \text{K}^{-1}$. Eleven terms are given in the expansion.

TABLE 2
RECENT POLYNOMIAL APPROXIMATIONS FOR $Q(\text{CO})^a$

Reference	Temperature Range (K)	Partition Function of CO
Gurvich <i>et al.</i> 1962	$293 < T < 6000$	$\log Q(\text{CO}) = 2.290 - 0.027\theta + 0.00031\theta^2 - 0.029\Lambda + 2.532/\theta - 2.098/\theta^2 + 1.231/\theta^3 - 0.258/\theta^4 - 0.162/\theta^5 + 0.116/\theta^6 - 0.021/\theta^7$
Gurvich <i>et al.</i> 1978	$500 < T < 6000$	$\log Q(\text{CO}) = 3.095 + 0.02262\theta - 0.000682\theta^2 - 1.0595\Lambda + 0.72133/\theta - 0.27823/\theta^2 + 0.05547/\theta^3$
	$1000 < T < 20,000$	$\log Q(\text{CO}) = 4.088 + 0.4028\theta - 0.01859\theta^2 - 4.0697\Lambda - 1.08196/\theta + 0.24836/\theta^2 - 0.01947/\theta^3$
Sauval 1972	$1000 < T < 9000$	$\log Q(\text{CO}) = 3.530 + 0.0832\theta - 1.936\Lambda$
Scalo and Ross 1976 ...	$1000 < T < 6000$	$Q = 57.003 + 217.39t + 103.29t^2 + 3.3576t^3 - 0.11388t^4 = 57.003 + 1095.6/\theta + 2623.7/\theta^2 + 429.85/\theta^3 - 73.480/\theta^4$
Irwin 1981	$1000 < T < 16,000$	$\ln Q = 162.048 + 105.132l - 26.513l^2 + 3.3203l^3 - 0.20485l^4 + 0.005014l^5$
Present work	$1000 < T < 9000$	$\log Q(\text{CO}) = 3.6076 - 1.7608\Lambda + 0.4172\Lambda^2$

^aSymbols used: T = temperature in kelvins; $t = T/1000$; $\theta = 5040/T$; $L = \log_{10} T$; $\Lambda = \log_{10} \theta$; $l = \ln T$; $\lambda = \ln \theta$.

This is rather larger than is ideal for computational purposes and may also give rise to quite spurious inflections. Slightly shorter expressions are given by Gurvich *et al.* (1978).

The polynomial in Sauval (1972) is based on equation (3) and is valid for a simplified molecular model. The "minimax" method (i.e., minimization of the maximum absolute errors) as described in Barrodale and Young (1966) was used rather than the method of least squares, because the accuracy so obtained is much higher.

The polynomial for Q proposed by Scalo and Ross (1976) needs all five coefficients at temperatures higher than 2500 K.

Irwin (1981) has proposed an analytical development with six numerical coefficients. His formula uses six numerical coefficients for all molecules, which, in some cases, is not always necessary for a given accuracy. Sarychev (1980) proposed the three-parameter formula $Q(T) = aT \exp(T/c)/[1 - \exp(-b/T)]$. This fits $Q(T)$ for CO quite well in the restricted temperature interval 3000–8000 K. Finally, Shankar and Littleton (1983) gave a five-parameter expansion in $\ln T$ for $\ln Q$ of ZrO. Their results agree with ours to better than 0.5% for $T \leq 4500$ K (fortunately the range where ZrO is important), but the difference increases to 14% at 8000 K.

a) Negative Molecular Ions

For negative ions, such as AB^- , we have assumed that the spectroscopic constants are identical with those of the neutral molecule AB , because in the few pairs for which data are available (Huber and Herzberg 1979), such as a C_2^- , C_2 and HS^- , HS , corresponding constants are not very different. Moreover, we have assumed that the ground states of isoelectronic molecules are the same (e.g., $X^3\Sigma^-$ of CH^- and NH), so that the ratio of the partition functions is approximately equal to the ratio of the electronic statistical weights of the ground states $g_e(AB^-)/g_e(AB)$.

b) Atomic Partition Functions

A large variety of polynomial representations of atomic partition functions have been proposed in the past. Let us quote some of them in order of increasing number of terms.

1. In de Galan, Smith, and Winefordner (1968), the following development is used with six terms, in the temperature range 1500–7000 K, for 73 elements:

$$Q(T) = \sum_{n=0}^5 a_n \left(\frac{T}{1000} \right)^n. \quad (5)$$

2. In the temperature range 3500–20,000 K another polynomial expression is proposed by Bolton (1970) for some elements and by Aller and Everett (1972) for rare earths:

$$\ln(Q - g_0) = \sum_{n=0}^5 a_n (\ln \theta)^n, \quad (6)$$

where g_0 is the electronic statistical weight of the ground state.

3. A similar development is used by Irwin (1981) for 92 elements in the range 1000–16,000 K:

$$\ln Q = \sum_{n=0}^5 a_n (\ln T)^n. \quad (7)$$

4. A quite different expression is given by Van Diest (1980), with a maximum of nine terms for rare earth elements in the temperature range 1000–9000 K:

$$Q = \sum_{n=0}^8 a_n C_n(t), \quad (8)$$

where $t = (T - 5000)/4000$ and $C_n(t)$ is the Chebyshev function defined by

$$C_n(t) = \cos(n \cos^{-1} t). \quad (9)$$

5. For the lightest elements (Traving, Baschek, and Holweger 1966, based on a method given by Schlender and Traving 1965), the following expression appears to fit atomic partition functions for a very large temperature range (100 K up to almost any temperature of practical interest), although large numbers of coefficients a_n, b_n are required:

$$Q = \sum_{n=0}^{n_{\max}} a_n 10^{-b_n \theta}. \quad (10)$$

6. The results of Gurvich *et al.* (1962) lead to a development, similar to that for molecules, in 11 terms in the temperature range 293–6000 K for many elements. An expression is given for the Gibbs energy function ϕ_T :

$$\phi_T = \sum_{n=-2}^7 a_n \left(\frac{T}{10000} \right)^n + b \ln \left(\frac{T}{10000} \right). \quad (11)$$

This function is related to the partition function Q by equation (4), whence

$$\log Q = \sum_{n=-2}^7 a'_n \left(\frac{T}{10000} \right)^n + b' \ln \left(\frac{T}{10000} \right). \quad (12)$$

Table 3 shows some of these series expansions in the case of iron. Except for results obtained by Van Diest (1980) and by Schlender and Traving (1965), the coefficients were calculated by the method of least squares.

In the limited temperature range chosen here, namely 1000–9000 K, we find that the following expression fits very well the calculated values of the partition function:

$$\log Q = \sum_{n=0}^4 a_n (\log \theta)^n. \quad (13)$$

An almost identical expansion in natural, rather than common logarithms, used by Bolton (1970), gives very similar results. Thus, the same polynomial expression has been adopted for both atoms and molecules. A total of 69 neutral atoms and 19 positive ions are considered here.

III. POLYNOMIAL EXPANSIONS FOR EQUILIBRIUM CONSTANTS

The determination of the equilibrium constant from atomic and molecular partition functions and from the dissociation energy is straightforward (see, e.g., Tatum 1966). The quantity pK is used throughout; i.e., the equilibrium constant is calculated in terms of partial pressures rather than number densities.

TABLE 3
RECENT POLYNOMIAL APPROXIMATIONS FOR $Q(\text{Fe})^a$

Reference	Temperature Range (K)	Partition Function of Fe
Bolton 1970	$3500 < T < 20000$	$\ln(Q - 9) = 2.930047 - 0.979745\Lambda + 0.760270\Lambda^2 + 0.118218\Lambda^3$
de Galan, Smith, and Winefordner 1968	$1500 < T < 7000$	$Q = 10.658 + 7.3013t - 2.2102t^2 + 0.45301t^3 - 0.040732t^4 + 0.0015017t^5$
Irwin 1981	$1000 < T < 16000$	$\ln Q = -1156.095 + 746.598t - 192.8657t^2 + 24.966t^3 - 1.6193t^4 + 0.042118t^5$
Traving, Baschek, and Holweger 1966	$50 < T < \infty$	$Q = 9 + 14.4102 \times 10^{-0.066\theta} + 2.7050 \times 10^{-0.339\theta} + 36.2187 \times 10^{-0.928\theta} + 22.8883 \times 10^{-1.679\theta} + \text{many more terms}$
Sauval 1972	$1000 < T < 9000$	$Q = 9 + 14.4572 \times 10^{-0.152\theta} + 2.7023 \times 10^{-0.8413\theta} + 37.4687 \times 10^{-2.1007\theta} + 534.7327 \times 10^{-6.53854\theta}$
Present work	$1000 < T < 9000$	$\log Q = 1.44701 - 0.6704\Lambda + 1.01267\Lambda^2 - 0.81428\Lambda^3$

^aFor symbols, see Table 2.

TABLE 4
RECENT POLYNOMIAL APPROXIMATIONS FOR $\log P K (\text{CO})^a$

Reference	Temperature Range (K)	$\log P K (\text{CO})$
Gurvich <i>et al.</i> 1962	$293 < T < 6000$	$13.50 - 11.165\theta - 0.0002\theta^2 - 2.458\Lambda - 2.431/\theta + 1.850/\theta^2 - 0.884/\theta^3 + 0.0411/\theta^4 + 0.227/\theta^5 - 0.1226/\theta^6 + 0.021/\theta^7$
Schadee 1968	$1700 < T < 5000$	$12.609 - 11.5065\theta + 0.0435\theta^2$
Kurucz 1970	$500 < T < 6000$	$13.75 - 11.108\theta - 2.5\Lambda - 3.459/\theta + 3.788/\theta - 2.606/\theta^3 + 0.744/\theta^4$
Sauval 1972	$1000 < T < 9000$	$12.544 - 11.4503\theta + 0.0403\theta^2 - 0.419\Lambda$
Tsuji 1973	$1000 < T < 6300$	$12.820 - 11.795\theta + 0.17217\theta^2 - 0.0229\theta^3 + 0.0011\theta^4$
Vardya 1966	$1000 < T < 6000$	$12.641 - 11.591\theta - 0.08885\theta^2 + 0.07347\theta^3$
Present work	$1000 < T < 9000$	$12.2263 - 0.8829\Lambda - 0.1230\Lambda^2 - 0.3226\Lambda^3 - 11.092\theta$

^aFor symbols, see Table 2. Quantity K in SI units (newtons per square meter).

Table 4 shows some proposed polynomials used in the past. The same general remarks given for molecular partition functions can also be applied here to the equilibrium constants. The expressions given in Table 4 have been modified, in some cases, from the expressions given in the original papers cited. For example, Gurvich *et al.* (1962) gave an expansion in which T was expressed in units of 10,000 K and $P K$ was in atmospheres, and in Kurucz (1970) $\log(1/K)$ was expanded as a polynomial in T . (Where applicable, we have converted published formulae for use with SI units.)

In addition to the expressions listed in Table 4, Tarafdar (1977) gave the following expression for some molecules:

$$\log P K = \sum_{n=0}^{n_{\max}} a_n \theta^n - \frac{2}{3} \log \theta, \quad | \text{by Tarafdar} \quad (14)$$

which is similar to that of Sauval (1972) except for the fixed coefficient of $\log \theta$.

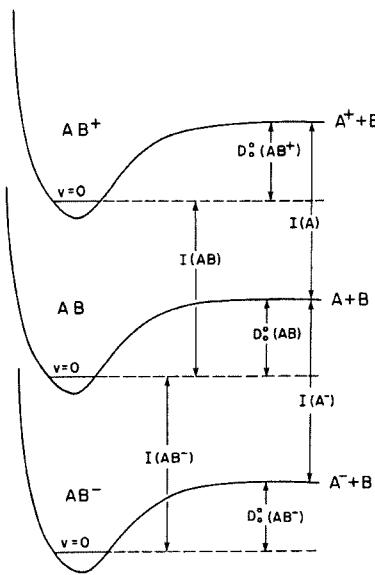


FIG. 3.—Illustrating the relations $D_0^0(AB^-) + I(A^-) = D_0^0(AB) + I(AB^-)$, $D_0^0(AB) + I(A) = D_0^0(AB^+) + I(AB)$. Potential curves are relative to the ground states of AB , AB^+ , and AB^- .

A further interesting approach has been suggested by Bohn and Wolf (1984) and applied to H_2 and CO. In their method the rotational and vibrational parts of the partition function are separated, thus much reducing the size of the computation. To compensate for the errors introduced by this procedure the authors supply correction factors in the form of two polynomial series in T . They believe that this gives smaller errors than a straightforward polynomial for Q . This seems to be a somewhat artificial approach, and in any case eight polynomial coefficients are needed, thus somewhat neutralizing the earlier saving in computation. However, the advantage claimed is that this technique leads to more accurate values of the temperature derivatives of the partition function in the computation of thermodynamical quantities.

Figure 2 shows $(\log^P K + \theta D_0^0)$ as a function of $\log T$ for the particular case of CO. As shown in Table 4, this can be represented well by a polynomial in $\log \theta$ (or in $\log T$) (see Table 4). We have found that this leads to the best fit with a minimum number of terms. Furthermore, the minimax method always leads to a smaller maximum error (especially near both limits) than the least-squares technique.

For positive molecular ions, Figure 3, which we hope will be self-explanatory, shows the relation between ionization potentials, I , and dissociation energies D_0^0 :

$$D_0^0(AB) + I(A) = D_0^0(AB^+) + I(AB), \quad (15a)$$

where the dissociation of AB^+ leads to A^+ and B , with $I(A) < I(B)$.

We have not tabulated equilibrium constants for negative molecular ions, but it is in any case easy to derive the ratio of number densities $n(AB^-)/n(AB)$. But first, a brief word on nomenclature is in order. The energy required to remove an electron from AB^- to form AB can hardly be correctly called the “ionization energy of AB^- ”, because removal of the electron does not create an ion! Instead this energy is called the *electron affinity* of AB , or the *neutralization energy* of AB^- . However, for consistency in notation we shall use

$I(AB) \equiv$ ionization energy of AB ;

$I(AB^-) \equiv$ electron affinity of $AB \equiv$ neutralization energy of AB^- ; since in each case the quantity is equal to the energy required to remove an electron from the species in parentheses.

Figure 3 also illustrates the following relation between electron affinities and dissociation energies:

$$D_0^0(AB^-) + I(A^-) = D_0^0(AB) + I(AB^-), \quad (15b)$$

where it is assumed that dissociation of AB^- leads to A^- and B and therefore $I(A^-) > I(B^-)$.

Moreover, the rotational and vibrational constants B_e , ω_e are very similar for the species AB and AB^- . However, the ground electronic state of AB^- is usually the same as the ground state of an isoelectronic neutral molecule. For example, NH is isoelectronic to CH^- . Since the ground state of NH is known to be ${}^3\Sigma^-$, it may be assumed that the ground state of CH^- is also

TABLE 5
COEFFICIENTS FOR MOLECULAR PARTITION FUNCTIONS AND EQUILIBRIUM CONSTANTS

MOL.	N	DO	EQUILIBRIUM CONSTANT					PARTITION FUNCTION							
			(EV)	B0	B1	B2	B3	B4	B5	MAX. ER.*	A0	A1	A2	A3	A4
LH	1	2.4287	9.9506	-0.5163	0.1833	-1.7211	1.2805	0.0031	*	3.2564	-2.1799	0.7236	-0.1052	0.0026	
BEH	3	2.6644	9.6592	-0.6592	-0.1929	-0.3299	-1.4246	0.6362	0.0033	*	3.2507	-2.0115	0.8852	-0.3258	0.0000
BBH	5	3.4200	10.5064	0.5064	0.1929	-0.3299	-1.4246	0.6362	0.0034	*	3.1862	-2.6821	0.5142	-0.6959	0.0056
CH	5	3.4650	10.5263	-0.5284	-0.7239	0.5713	0.0027	*	3.3586	-2.0656	0.9624	-0.2349	0.0008		
NH	4	3.400	10.4609	-0.7387	-0.5713	0.0034	*	3.0735	-1.8501	0.9607	-0.3935	0.0019			
O	2	4.3920	10.7881	-0.8762	-0.5436	0.0022	*	3.0929	-1.6778	0.6743	-0.1874	0.0007			
H	F	1	5.8690	11.2835	-0.9228	-0.5642	0.0164	*	3.4164	-1.6132	0.6357	-0.1677	0.0008		
NAH	3	1.8800	9.7127	-0.3175	0.2445	-2.4962	2.0335	0.0053	*	3.5453	-2.3457	0.8557	-0.1685	0.0032	
MG	4	1.3400	9.2846	-0.3587	-0.1220	-1.5627	1.3047	0.0034	*	3.6704	-2.2682	0.9354	-0.2597	0.0011	
ALH	4	3.0600	10.3999	-0.0733	-1.6121	0.0063	0.7650	0.0058	*	3.3209	-2.5909	1.7415	-0.7636	0.0057	
SIH	2	3.0600	10.2379	-0.7143	-0.6404	0.1156	0.0031	*	3.6903	-1.9801	0.7704	-0.2247	0.0021		
PH	4	3.0200	10.1061	-0.7236	-0.2853	-0.2032	0.0014	*	3.4957	-2.0871	0.9617	-0.2598	0.0007		
S	3	3.5500	10.4145	-0.8190	-0.5524	0.0203	0.0014	*	3.4935	-1.8385	0.5852	0.0036			
H	C _L	1	4.4336	10.9013	-0.8274	-0.5974	0.0025	*	2.8005	-1.7476	0.5310	0.0024			
K	H	1	1.8600	9.5373	-0.6621	1.4043	-3.7901	2.5004	0.0034	*	3.7667	-2.2837	0.5043	0.1196	
CAH	9	1.7000	9.1952	-0.8802	1.6160	-2.5221	1.3114	0.0015	*	3.8411	-2.3891	1.3578	-0.6893	0.0051	
CRH	2	2.5000	9.8937	-1.2266	1.1519	-1.9385	0.9790	0.0025	*	4.0929	-2.2491	0.8923	-0.1787	0.0042	
MNH	2	2.5000	9.8587	-0.8607	0.7116	-2.8120	1.8126	0.0028	*	4.1860	-2.1839	0.8747	-0.2513	0.0031	
COH	2	10.3877	-0.8745	-0.0412	-1.7427	1.4621	0.0022	*	4.1047	-2.2620	0.4803	0.2721	0.0016		
NH	4	3.0700	10.7821	-0.4987	-1.0040	0.3197	0.0037	*	3.6736	-2.3271	1.0818	-0.5338	0.0037		
CUH	3	2.7300	10.2359	-0.8631	-0.2045	0.5079	-0.7366	0.0027	*	3.1001	-2.1456	1.1944	-0.5914	0.0054	
ZNH	4	0.8510	9.3436	-0.3528	-0.866	-1.2327	0.8192	0.0005	*	3.6197	-2.1349	0.3017	0.3458	0.0035	
GAH	3	2.8400	10.3713	-0.3071	-1.3737	0.0238	0.5134	0.0055	*	3.3100	-2.3703	1.4724	-0.7575	0.0006	
GEH	2	3.3000	10.0536	-0.8571	-0.8573	0.0013	*	3.7954	-2.0472	0.6234	0.0036				
ASH	1	3.6000	10.1156	-1.1074	0.3885	-0.5746	0.0019	*	3.5022	-1.7207	0.3759	0.0036			
SEH	1	3.2000	10.2854	-1.1036	-0.3013	0.0017	*	3.5571	-1.6887	0.3912	0.0031				
H	BR	1	3.7280	10.7059	-0.8545	-0.5918	0.1995	0.0012	*	3.9255	-1.8051	0.5439	0.0023		
RBH	2	1.66600	9.1300	-1.0867	1.9505	-3.5983	1.8586	0.0025	*	3.8516	-2.2990	0.4213	0.2106	0.0029	
SRH	6	10.0979	-2.2770	-0.7461	0.1382	2.2686	0.0025	*	3.9406	-2.3979	1.2564	-0.5865	0.0058		
PDH	1	2.2800	10.0411	-0.4123	-0.7461	0.1382	0.0015	*	3.3378	-1.7316	0.3697	0.0037			
AGH	6	0.6780	9.2759	-0.4191	-0.6388	0.1624	0.0029	*	3.2501	-2.0994	0.8105	-0.2140	0.0011		
CDH	4	2.4800	10.1447	-0.3957	-1.7087	0.5557	0.5123	0.0044	*	3.6916	-2.0809	0.6389	-0.1625	0.0030	
INH	4	2.7300	9.8503	-1.4863	-0.6936	0.3966	0.0036	*	3.4418	-2.4303	1.4516	-0.6835	0.0047		
SNH	1	9.9235	-1.0973	0.4311	-0.4708	0.0032	*	3.8321	-1.7739	0.3402	0.0041				
SBH	1	10.0053	-1.0836	-0.0154	-0.1301	0.0017	*	3.7208	-1.7994	0.3179	0.0041				
TEH	1	3.0541	10.4946	-0.7350	-0.4527	0.02384	0.0025	*	3.7592	-1.7365	0.3667	0.0037			
H	I	1	1.8100	9.4674	-1.1765	0.9753	-0.5222	2.6745	0.0048	*	3.1038	-1.8753	0.5591	0.0052	
CSH	4	1.9500	9.2562	-0.9600	-1.9128	2.8211	3.7826	-6.1227	0.0101	*	3.9070	-2.2534	0.3373	0.2409	0.0028
BAH	9	1.5500	10.5707	-2.0868	0.6501	-0.3842	0.0029	*	4.1275	-3.4445	3.4729	-1.6164	-0.6508		
LAH	15	1.9300	9.1165	-0.8337	2.3885	-6.1903	4.1950	0.0063	*	3.8992	-2.3556	1.0469	-0.3525	0.0040	
YBH	1	1.4800	10.5855	-0.8305	-0.9753	0.7861	-0.6278	0.0048	*	3.4069	-2.0439	0.5556	0.0035		
PTH	6	3.2200	10.3037	-1.0665	-0.0737	0.4760	-0.7257	0.0012	*	3.6862	-2.0426	1.1143	-0.5023	0.0045	
AUH	2	0.3744	9.2184	-0.5946	0.1954	-0.5625	0.0023	*	3.0567	-1.9182	0.7472	-0.2103	0.0020		
HGH	3	1.9700	9.8718	-0.4509	-0.8717	0.5256	-0.0995	0.0021	*	3.7548	-1.9107	0.1771	0.5461	0.0020	
T LH	1	1.5900	9.1386	-0.9871	-0.4793	1.3671	-1.1166	0.0042	*	3.4888	-2.4274	1.2776	-0.4865	0.0054	
PBH	3	2.9000	9.6707	-0.2999	-0.2473	-1.0153	0.6873	0.0040	*	4.0319	-2.4374	1.4150	-0.5829	0.0058	
BITH	3	1.8450	10.1667	-0.4814	-0.6444	-0.7916	0.8534	0.0015	*	3.9222	-2.3670	0.8067	0.0038		
HEH	+	1	3.1400	9.7188	-0.7267	0.0041	-1.0889	0.7404	0.0010	*	2.3613	-1.9733	0.6761	0.0794	0.0060
BEH	+	2								2.8899	-1.9119	0.5829		0.0036	

TABLE 5—Continued

MOL.	N	DO	EQUILIBRIUM CONSTANT					PARTITION FUNCTION					MAX. ER.*	
			B0	B1	B2	B3	B4	B5	A0	A1	A2	A3	A4	
B	2	1.9500	10.3048	-0.7004	-0.5C24									0.0020
C	4	4.0850	10.7018	0.0994	-1.4610	-0.8279	1.3625							0.0038
N	4	3.3900	9.6574	-0.6294	-0.6294	0.1927								0.0040
H	3	5.01900	10.4950	-0.6799	-0.9224	0.3310								0.0034
F	2	3.0230	10.6684	-0.6549	-0.9526	0.2645								0.0012
NE	1	2.0800	10.1080	-0.8691	-0.4086									0.0022
MG	2	2.0800	9.4108	-0.5435	0.0987	-1.7288	1.3461							0.0039
AL	2	3.1700	9.7925	-0.7214	0.4948	-0.8627								0.0031
SI	2	2	10.5758	-0.7532	-0.6480	0.1410								0.0027
P	1	3.5600	9.7604	-1.1045	0.3654	-0.5871								0.0033
S	1	3.8800	10.2741	-0.9924	-0.2456	-0.2060								0.0026
H	CL+	2	4.6530	10.4094	-0.8021	-0.6304								0.0018
ZN	H	2	2.0000	9.5271	-0.4794	-0.5934								0.0014
H	BR+	2	3.68940	10.2047	0.9225	0.5992	0.2723							0.0016
CD	H	2	2.0000	9.4122	-0.4222	-0.6361								0.0037
HG	H	1	2.9930	9.5121	-0.5024	-0.6184								0.0041
C	N	3	7.6600	11.4479	-0.4840	-0.4160	-0.9435	0.8380						0.0033
CD	N	2	11.0920	12.2263	-0.8829	-0.1230	-0.3226							0.0024
C	F	3	5.6700	11.1538	-0.6431	-0.4255								0.0037
SI	C	1	4.6400	10.8445	-0.9184	0.1532	-0.3771							0.0038
C	S	4	5.8800	11.0579	-0.4737	-0.1729	-1.2021	C.5631						0.0044
C	S	4	7.1550	11.8298	-0.8130	-0.5170	1.1553	-1.0249						0.0030
C	CL	2		10.7975	-0.5818	-0.3397								0.0034
C	SE	2	5.9800	11.6323	-0.8887	-0.4754	0.8627	-0.7308						0.0053
C	BR	1	4.1100	10.5031	-0.8128	0.0167								0.0025
RH	C	4	6.0100	11.8689	-1.0481	-0.5630	0.3225							0.0014
IR	C	4	6.4500	11.6317	-1.0444	0.0162								0.0028
PT	C	4	6.2800	12.0345	-0.6227	-0.8549	0.2473							0.0039
C	N	3	4.8500	12.0523	-0.3741	-0.6714	-0.7355	C.6846						0.0043
C	O	2	8.3280	11.5907	-0.7647	-0.4319								0.0029
B	N	2	10.6476	-0.6812	-0.958	-0.3121								0.0025
N	O	2	6.4968	11.2253	-0.8143	0.0446	-0.4529							0.0019
N	F	3	3.5000	10.8509	-0.5611	-0.4198								0.0019
AL	N	2	10.1571	-0.5225	-0.4462	-0.2266								0.0035
SI	N	6	11.0504	-0.4223	-0.6714	-0.6714								0.0023
P	NN	2	6.3600	11.2316	-1.0411	0.6714	-0.8076							0.0026
N	S	5	4.8000	10.9036	-0.7786	0.0941	-0.3808							0.0019
N	CL	2	10.1571	-0.6697	-0.0703	-0.2794								0.0024
TIN	N	1	4.9000	11.7421	-1.7267	1.5855	-1.3639							0.0041
AS	N	1	4.11252	-0.9863	0.6970	-0.7720								0.0023
N	SE	6	4.0000	10.7173	-0.6078	-0.4482	0.3251							0.0064
ZR	N	1	5.8100	11.6496	-1.8280	0.8730	-0.7237							0.0038
NB	N	1	10.9506	11.6210	-0.8373	0.0676	-1.0507	0.6864						0.0038
N	S	+	6.3000	11.2307	-0.8277	0.5112	-1.3707	0.7033						0.0024
L1	O	2	3.1900	10.0377	-0.4691	0.7661	-2.2854	1.395						0.0020
BE	O	6	4.6000	10.6366	0.5176	-0.4647	-3.7714	3.3677						0.0016
B	O	4	8.2800	11.6221	-0.7011	-0.4788								0.0035
F	O	1	2.2300	11.0588	-0.6355	-0.2688	-0.1683							0.0033
NA	O	1	2.6000	10.0152	-0.8008	1.1032	-2.6609	1.7389						0.0018
									5.3711	-1.9284	0.1449		0.0026	

TABLE 5—Continued

MOL.	N	STATES	DG (EV)	EQUILIBRIUM CONSTANT						PARTITION FUNCTION						MAX. ER.*
				B0	B1	B2	B3	B4	B5	MAX. ER.*	A0	A1	A2	A3	A4	
MG	0	7	3.5300	9.7780	-0.0290	1.1725	-1.1724	-0.2742	-0.4863	0.9291	0.0040 *	5.3182	-2.6502	-0.2781	-0.7823	1.3157
AL	0	6	5.2700	10.9663	0.0703	-0.2742	-0.8349	-0.5248	1.1271	-1.1984	0.0008 *	4.9191	-6.6291	0.5831	0.3163	0.0042
SI	0	10	8.2600	11.8772	-0.3876	-0.8349	-0.9497	0.3972	-0.5660	0.0032 *	4.2275	1.9144	0.7201	-1.3099	1.1657	0.0035
P	0	4	6.1500	10.9660	-0.9497	0.3972	-0.5660	0.0031 *	4.8326	-1.9182	0.3582	0.0019				
S	0	3	5.3590	11.3119	-0.5729	-0.3278	-0.2574	0.0011 *	4.7963	-2.1308	0.5224	0.0014				
CL	0	4	2.7505	10.8756	-0.5189	-0.3876	-0.2574	0.0025 *	5.0025	-2.1026	0.4208	-0.1725	0.0023			
K	0	1	4.7600	10.1915	-1.0847	1.9449	-3.4048	1.8810	2.6646	1.9124	0.0060 *	5.0437	-3.4848	0.9872	2.7775	-2.6956
CA	0	6	4.9600	11.2335	0.1684	1.8170	-6.3417	2.6646	1.9124	0.0042 *	4.8065	-2.2129	0.9991	-0.5414	0.0037	
SC	0	4	6.8700	11.5015	-1.1288	0.8607	-0.9294	0.6478	-0.6737	0.0027 *	5.0351	-2.3739	0.8940	-0.3641	0.0020	
Tl	0	15	6.8700	11.4047	-1.1288	0.8607	-0.9294	0.6478	-0.6737	0.0021 *	5.0687	-2.2186	0.9545	-0.4592	0.0021	
V	0	4	6.4100	11.8610	-1.1543	0.3537	-0.4292	0.4416	-1.1862	0.0025 *	5.5270	-2.1311	0.6523	-0.2533	0.0021	
CR	0	2	4.4000	10.7452	-1.4464	1.3892	-2.9384	1.7034	0.0018 *	5.3855	-2.0226	0.3621	0.0038			
MN	0	2	3.7000	10.6819	-0.9413	1.3892	-2.9384	1.7034	0.0018 *	5.0235	-2.0440	0.5065	0.0012			
FE	0	3	4.2000	11.1428	-1.3307	0.5711	-0.0411	0.6667	-0.4076	0.0042 *	4.9367	-1.9163	0.1656	0.0029		
Ni	0	1	3.8700	11.8158	-0.9732	0.7120	0.3346	-0.3684	-0.0939	-1.1012	0.7611	0.0021 *	5.3500	-2.3114	0.7400	-0.4122
Cu	0	6	2.7900	10.2956	-0.6736	-0.6891	-0.9142	-1.0323	-1.3596	-1.2339	1.0515	0.0023 *	4.9645	-2.0340	0.3183	0.0026
GA	0	2	3.9100	11.0366	-0.0939	-0.8939	-1.0122	-1.0323	-1.0596	-1.0546	0.0196	0.0024 *	4.4855	-2.0441	0.9719	1.6102
GE	0	5	6.7800	11.6762	-0.9142	-1.0367	-1.1101	-0.6405	-0.5930	0.0196	0.0024 *	5.0509	-2.1235	0.2440	0.0023	
AS	0	6	4.9800	11.9016	-0.7982	0.4555	-0.0196	-0.5465	0.4226	0.0027 *	5.0293	-2.2137	0.8127	-0.4546	0.0035	
SE	0	7	4.4100	11.1518	-0.6351	-0.6997	0.4226	0.4693	-0.1983	0.0164	0.0028 *	5.2352	-2.2395	0.2781	0.0035	
BR	0	3	2.3970	10.7396	-1.1054	1.7616	-2.7337	1.2892	1.0515	1.0515	0.0021 *	5.0676	-2.1221	1.5631	1.8476	-2.3506
Rb	0	1	4.8800	10.2479	-0.1054	1.8976	-6.3299	3.0605	1.0515	0.0066 *	5.1657	-3.5194	1.5631	1.8476	-2.3506	
SR	0	6	7.2900	11.4412	-1.3967	1.1101	-0.6405	-0.5930	0.0053 *	4.9515	-2.0866	0.6565	-0.3082	0.0038		
Y	0	4	7.8500	11.5031	-1.1916	0.5692	-0.1795	0.6954	-0.9700	0.0039 *	5.3279	-2.4694	0.2164	-0.2313	0.0039	
ZR	0	17	7.8500	11.9070	-1.5994	0.6954	-0.9700	0.6020	-0.4302	0.0011 *	5.1386	-1.9248	0.2897	0.0027		
NB	0	1	7.8000	11.4963	-1.6269	0.6020	-0.4302	0.3504	-0.2994	0.0024 *	5.3642	-1.8834	0.2173	0.0023		
RU	0	1	5.3000	11.4963	-1.6269	0.6020	-0.4302	0.3504	-0.2994	0.0037 *	5.6400	-2.2738	0.4857	-0.1403	0.0020	
AG	0	6	2.2900	9.9937	-0.2994	-0.3504	-0.9163	-0.4423	0.1520	0.0024 *	5.1354	-1.9915	0.2609	0.0013		
IN	0	1	2.9400	10.8195	-0.9163	-0.2465	-0.9836	0.6380	0.7103	-0.2787	0.0028 *	5.7103	-2.0718	0.6368	-0.3377	
SN	0	4	5.4900	11.3457	-1.2070	-1.5994	-0.6968	0.2752	0.4120	-0.9811	0.0025 *	5.1963	-2.3071	0.4144	-0.3734	
SB	0	5	4.3900	10.8248	-0.6968	0.2752	0.4120	-0.9811	0.0669	0.0039 *	5.2844	-2.1005	0.1946	0.0023		
TE	0	2	3.9000	10.8627	-0.7738	0.6669	-0.1963	-0.2107	-0.1972	3.6491	0.0037 *	5.3109	-2.3921	0.4198	0.0023	
I	0	3	1.8000	10.6616	-0.2700	-0.2107	-0.1972	-0.1972	-0.1972	3.6491	0.0019 *	5.1001	-2.6335	2.1625	-2.0727	
BA	0	7	5.7900	10.8582	-1.8538	-0.1005	-0.3408	-0.4067	0.6561	0.0147	5.1147	-2.0516	0.3135	0.0065		
LA	0	10	8.2300	11.6727	-1.4495	-0.1148	-0.7551	0.8494	1.3151	0.0019 *	5.406	-1.8832	0.2178	0.0033		
CE	0	1	8.1800	12.2040	-2.5463	0.1737	0.2227	0.2227	0.2227	0.0028 *	5.2774	-1.8882	0.2103	0.0036		
TB	0	1	7.1900	12.3059	-2.0468	0.8646	-0.4632	0.4146	-1.3218	0.9452	0.0015 *	4.9940	-2.0768	0.5113	0.0047	
LU	0	4	1.8000	11.3207	-1.1864	-0.5389	-0.3026	-0.1607	0.3408	0.0039 *	4.6051	-2.1287	0.9011	-0.5178		
HF	0	7	8.1900	11.9286	-1.5389	-0.1005	-0.4067	0.6561	0.0028 *	5.1001	-2.8433	1.738	0.5173	-0.8561		
TA	0	8	8.2000	11.5041	-1.1746	-0.2797	-0.4810	1.3151	0.1727	0.0036 *	5.1129	-1.8799	0.2718	0.0035		
W	0	1	6.8000	11.3448	-2.0836	0.1727	-0.4810	0.4378	0.4378	0.0023 *	5.2391	-2.0423	0.5144	-0.1725		
IR	0	2	3.6400	11.4550	-1.3926	0.0274	0.7416	-0.6759	0.0274	0.0023 *	4.6742	-2.0805	0.5153	-0.2019		
PT	0	2	3.8200	11.9957	-0.8149	-0.3026	-0.1607	0.3408	0.0033 *	4.8510	-2.3241	1.3926	-1.6743	0.0016		
PB	0	4	3.8300	10.7139	-1.1615	-0.3056	-2.4034	-2.2780	0.0013 *	5.2349	-2.5169	1.2737	-0.6580	0.0027		
BI	0	6	3.4700	10.7684	-0.2412	-0.6923	0.1559	0.4378	0.4378	0.0023 *	4.9201	-2.8341	1.2323	-0.1963		
TH	0	12	9.0000	11.8865	-1.6229	-0.1214	0.4378	0.4378	0.4378	0.0026 *	3.6885	-1.7629	0.3487	0.0049		
B	0	+	1	11.5579	-0.7733	-0.0834	-0.3266	0.0834	0.0834	0.0026 *	4.5010	-1.8318	0.2842	0.0041		
SI	0	+	1	4.9800	11.2473	-0.8817	0.0457	-0.3613	0.5314	-0.6840	0.0020 *	4.1845	-1.8326	0.3220	0.0038	
P	0	+	1	8.4100	11.2658	-0.9964	0.5314	-0.6840	0.0181	-0.3788	0.0007 *	4.7517	-1.8175	0.2998	0.0041	

TABLE 5—Continued

MOL.	N	STATES	DD (EV)	EQUILIBRIUM CONSTANT					PARTITION FUNCTION					MAX. ER.	
				B0	B1	B2	B3	B4	B5	A0	A1	A2	A3	A4	
AS	0	+	2	11.1821	-0.9353	0.5125	-0.6106			0.0015	*	4.04220	-1.9221	0.3190	0.0024
TA	0	+	2	11.4231	-0.0246	0.461	-0.1376	0.0831		0.0022	*	4.03366	-1.9527	0.3536	0.0019
LI	F	1	5.9100	10.6814	-0.5892	0.2241	-1.3376			0.0020	*	4.01338	-0.21584	0.6294	-0.1988
BE	F	4	5.08500	10.3864	-0.7484	0.1660	-0.5775			0.0043	*	4.02335	-1.9614	0.4093	0.0024
BF	2	7.8100	11.5877	-0.5738	-0.5283					0.0036	*	3.08557	-1.9713	0.5889	-0.1808
NA	F	1	5.3300	10.4112	-0.4247	0.4866	-2.4486	1.0135		0.0051	*	4.08566	-2.2801	0.5730	-0.1449
MG	F	4	4.7500	10.0433	-0.5350	0.2486	-1.4962	1.0741		0.0027	*	4.09332	-2.1380	0.5065	0.0025
AL	F	7	6.8900	11.2299	-0.4816	0.4865				0.0030	*	4.05405	-2.1033	0.6208	0.0016
SI	F	4	5.5700	10.9012	-0.6898	-0.3675				0.0037	*	5.00871	-2.0375	0.4478	0.0044
P	F	6	10.6706	-0.6432	-0.0481	-0.2458				0.0031	*	5.01446	-2.0268	0.6802	-0.2215
S	F	5	3.3000	10.6907	-0.5464	0.2122				0.0027	*	5.03092	-2.1406	0.1786	0.0019
CL	F	2	2.6173	11.1734	-0.0830	-1.6190	0.7791	0.1202		0.0056	*	4.06390	-2.5206	1.5058	-0.8835
K	F	1	5.0700	10.2876	-0.7142	1.4151	-3.3953	2.01866		0.0030	*	5.01495	-2.2814	0.4132	0.0039
CA	F	8	5.4800	9.9724	-1.0667	5.5919	-2.3638	0.9265		0.0034	*	5.02010	-2.2653	0.8941	-0.5384
SC	F	9	6.1700	10.5981	-1.0171	1.1437	-0.8442	-0.1190		0.0044	*	5.06041	-2.3100	0.6409	-0.5196
MN	F	2	4.3500	10.3577	-0.9194	1.4158	-2.9550	1.7349		0.0018	*	5.06080	-2.0214	0.2692	0.0020
FE	F	1	11.2390	-1.0958	0.8629	-1.7929	0.9010		0.0015	*	5.03670	-2.0615	0.1453	0.1975	
N	I	1	11.6924	-0.9714	-0.025	-0.3389				0.0036	*	4.09604	-1.8995	0.1930	0.0033
CU	F	4	4.4200	10.7113	-0.7175	0.0832	-0.2180			0.0037	*	4.08370	-2.2884	0.8728	-0.4688
ZN	F	1	10.1169	-0.5424	-0.1226	-0.2252				0.0027	*	5.0622	-2.0212	0.2605	0.0037
GA	F	2	5.2800	11.0703	-0.6115	-0.4239	-0.1917			0.0025	*	4.08351	-2.1309	0.5213	-0.2157
GE	F	3	5.0000	10.7351	-0.7351	-0.092				0.0041	*	5.03375	-2.2045	0.3369	-0.1743
AS	F	6	4.2000	10.5800	-0.6139	-0.1061	0.3669	-0.5674		0.0027	*	5.02767	-2.2834	0.7368	-0.3787
SE	F	1	3.2100	10.7906	-0.9333	-0.5573				0.0022	*	5.02954	-1.8972	0.1966	0.0033
BR	F	3	2.5480	11.0229	-0.1654	-1.5765	1.1875	-0.1602		0.0054	*	4.08590	-2.5308	1.5162	-0.9432
RB	F	1	5.0000	10.2442	-0.7236	1.0207	-2.849	1.8249		0.0021	*	5.03264	-2.2828	0.3908	0.0036
SR	F	5	5.5800	9.9281	-1.2447	2.2363	-3.2305	1.3573		0.0038	*	5.03982	-2.3020	0.8817	-0.5139
Y	F	11	6.2000	10.6024	-1.0490	1.1985	-0.1664	-0.7350		0.0052	*	5.06990	-2.4244	0.4447	-0.5689
AG	F	1	3.6400	10.4871	-0.3791	-0.4005				0.0023	*	5.05659	-2.1695	0.4621	-0.1498
CD	F	1	3.2000	9.9569	-0.6087	-0.032				0.0034	*	5.02937	-1.9271	0.1470	0.0012
IN	F	3	5.2500	10.8279	-0.6921	0.9794	0.6273			0.0015	*	5.03952	-2.1957	0.6318	0.0026
SN	F	3	4.9000	10.5104	-0.9423	-0.8303	0.4075			0.0016	*	5.03928	-2.1924	0.1553	0.0041
SB	F	4	4.4000	10.5298	-0.5245	0.1505	-0.0979			0.0015	*	5.04569	-2.3562	0.3650	-0.2118
I	F	3	2.8790	10.8583	-0.1890	-2.3819	0.7919	4.3837	-4.3614	0.0040	*	5.04031	-2.4107	0.4508	-0.2583
CS	F	1	5.1500	10.2669	-0.2115	2.4490	-3.5500	1.4989		0.0037	*	5.0315	-2.9055	2.1344	-1.3055
BA	F	9	6.0500	10.1600	-2.0267	0.7124	3.0679	-3.4197		0.0060	*	5.04037	-2.2654	0.3684	0.0012
LA	F	1	11.7253	-2.0523	0.6883	-0.3671				0.0055	*	5.05142	-2.4761	1.2354	-0.7552
HO	F	1	11.3855	-0.9423	-0.8303	0.4075				0.0028	*	5.03974	-1.9224	0.1553	0.0041
Y5	F	4	4.8000	9.9282	-1.0348	3.0140	-6.3465	4.0162		0.0012	*	5.04368	-2.0523	0.2925	0.0022
LU	F	6	1.1.2570	-0.9729	-0.1425	-0.5448	0.5895			0.0049	*	5.04001	-2.4107	0.4508	-0.2583
HG	F	1	1.8000	9.8844	-0.4512	-0.0824	-0.2834			0.0017	*	5.09710	-2.2379	1.1483	-1.3055
TL	F	3	4.5700	10.5151	-0.7422	-0.1678	-0.7394			0.0032	*	5.04072	-2.0889	0.0694	0.300
PB	F	3	3.6400	10.0314	-1.1454	0.2111	1.3119	-1.4696		0.0009	*	5.01643	-2.1992	0.5398	-0.2303
LINA	I	1	9.0737	-0.5315	2.3446	-5.3446	3.4409			0.0027	*	5.04584	-2.3244	0.7267	-0.5992
AUST	I	3	3.2400	9.9729	-0.9545	0.5857	0.1695	-0.8312		0.0032	*	5.03162	-2.3170	-0.2319	0.6184
AS	P	2	10.8905	-1.1459	1.0654	-0.237	-0.4253			0.0013	*	6.01485	-2.2354	0.1414	0.0034
SB	P	1	3.6800	10.7736	-1.1956	1.0636	-0.3134	-0.5643		0.0039	*	5.00912	-2.0238	0.2672	0.0025
BE	S	4	3.8000	10.4512	-0.0175	-0.6182	-1.5058	1.4841		0.0034	*	5.03090	-2.0455	0.2420	0.0017
B	S	3	6.0100	11.2320	-0.5508	-0.8565	0.8903	-0.6407		0.0009	*	4.04452	-2.7285	1.4078	-0.4308
MG	S	2	2.4000	10.2940	-0.6300	0.4199	-1.5174	1.0037		0.0025	*	5.00367	-2.1625	0.4859	-0.1780

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TABLE 5—Continued

MOL.	STATES	DO (EV)	EQUILIBRIUM CONSTANT					PARTITION FUNCTION					MAX. ER.*			
			B0	B1	B2	B3	B4	B5	A0	A1	A2	A3	A4			
AL S	4	3.8400	10.8924	-0.5704	-0.3551	-0.2837	-0.2028	-0.1414	0.0031	* 5.2461	-2.1319	0.5340	-0.2309	0.0029		
SI S	1	6.4200	11.5515	-0.8733	0.0208	-0.2626	0.0040	* 4.8026	-1.9753	0.2600	0.0017	0.0036	0.0016	0.0022		
P S	5	4.5400	10.6659	-0.9384	-0.5114	-0.4560	0.0553	0.0043	* 5.2645	-2.0356	0.2168	0.0014	0.0018	0.0015	0.0022	
CA S	2	3.4600	10.3046	-1.2540	2.1302	-3.0765	1.2869	0.0040	* 5.4061	-2.0980	0.490	-0.1602	0.0019	0.0018	0.0016	
SC S	2	4.9200	11.2016	-1.3356	1.4964	-1.4560	0.0553	0.0039	* 5.8948	-2.2183	0.5928	-0.3106	0.0015	0.0015	0.0015	
TI S	6	4.7500	11.1227	-1.4043	0.9862	-0.7360	0.0144	-0.1618	0.0035	* 6.0763	-2.0602	0.3000	0.0020	0.0021	0.0019	
CR S	2	3.3700	10.5156	-1.6188	-1.6144	-1.4166	0.0009	1.4933	-2.8376	1.5845	0.0015	0.0015	0.0015	0.0015	0.0015	
MN S	2	2.8500	10.4506	-1.0009	1.4933	-2.8376	1.5845	0.0015	* 5.9355	-2.0621	0.3576	-0.1336	0.0020	0.0020	0.0016	
CU S	3	2.8000	10.1393	-0.9778	0.9007	-0.7035	0.0009	0.0007	0.0023	* 5.8410	-2.1481	0.1583	0.0016	0.0016	0.0016	
GE S	1	5.6700	11.3974	-1.0450	-0.2535	-0.2691	0.0024	* 5.1235	-2.0123	0.2327	0.0011	0.0011	0.0011	0.0011	0.0011	
AS S	2	10.5565	-0.9360	0.3232	0.1437	-0.6247	0.0026	* 5.6179	-2.0119	0.480	-0.1964	0.0030	0.0030	0.0030	0.0030	
SE S	4	3.7000	10.9106	-0.8288	-0.2802	0.2420	0.0042	* 5.4962	-2.1220	0.2729	0.0017	0.0017	0.0017	0.0017	0.0017	
SR S	2	3.4800	10.2823	-1.5340	2.9746	-3.5940	1.6135	0.0049	* 5.5570	-1.9342	0.1345	0.0025	0.0025	0.0025	0.0025	
YN S	1	5.4500	11.1927	-1.6274	1.7629	-0.2377	0.0054	* 5.7277	-2.1079	0.4253	-1.1323	0.0017	0.0017	0.0017	0.0017	
TE S	2	3.5000	10.6250	-0.8142	0.1980	0.4986	-0.6719	0.0005	* 5.9071	-2.0347	0.1216	0.0014	0.0014	0.0014	0.0014	
HA S	4	4.3600	10.5005	-1.8227	0.1931	2.5675	-0.7377	-2.0641	0.0063	* 5.6482	-2.7554	1.8050	-1.1323	0.0025	0.0025	0.0025
LA S	2	5.9100	11.4495	-1.9869	0.5209	-0.2144	0.0013	* 5.7277	-2.1079	0.4253	-0.1774	0.0017	0.0017	0.0017	0.0017	
PB S	4	3.4900	10.4773	-0.5003	2.7897	-2.4801	0.0034	* 5.5022	-2.4824	1.6002	-1.7951	0.7852	0.0027	0.0027	0.0027	
BI S	2	3.1700	10.2889	-0.5804	-0.1945	0.0313	0.0035	* 6.1258	-2.2747	0.7288	-0.3968	0.0025	0.0025	0.0025	0.0025	
L1 CL	1	4.8400	10.3223	-0.5527	0.2688	-1.5692	1.1464	0.0025	* 4.5605	-2.2216	0.5760	-0.1706	0.0016	0.0016	0.0016	
BE CL	3	10.0091	-0.6903	0.0756	-0.4330	0.0036	* 4.6966	-2.0541	0.4801	-0.1525	0.0029	0.0029	0.0029	0.0029	0.0029	
B CL	3	5.5000	11.1693	-0.4633	-0.9362	1.0561	-C.7173	0.0009	* 4.4084	-2.1648	0.8845	-0.5054	0.0061	0.0061	0.0061	
NA CL	1	4.2300	10.1005	-0.3434	0.7696	-3.0544	2.3313	0.0047	* 5.3364	-2.2844	0.2820	0.1185	0.0044	0.0044	0.0044	
MG CL	3	3.2906	9.7146	-0.5162	0.2041	-1.1277	1.1064	0.0028	* 5.4360	-2.1924	0.5172	-0.2163	0.0018	0.0018	0.0018	
AL CL	4	5.1206	10.8455	-0.3966	-0.7300	0.1184	0.0034	* 5.1115	-2.2303	0.8001	-0.5192	0.0016	0.0016	0.0016	0.0016	
SI CL	4	10.5520	-0.6176	0.3907	0.1592	0.0033	* 5.6255	-2.1497	0.478	-0.2454	0.0027	0.0027	0.0027	0.0027		
P CL	2	10.3949	-0.8014	0.2807	-0.4320	0.012	* 4.4901	-2.0810	0.3024	0.0114	0.0114	0.0114	0.0114	0.0114		
K CL	1	4.3400	9.9705	-0.7106	1.6598	-3.9857	2.6197	0.0030	* 5.6860	-2.3016	0.2086	0.1763	0.0049	0.0049	0.0049	
CA CL	8	4.0900	9.6477	-1.0163	1.5882	-2.6090	1.2516	0.0026	* 5.7494	-2.3340	0.6685	-0.5306	0.0037	0.0037	0.0037	
SC CL	5	3.4000	11.6024	-0.9624	0.6696	-0.7441	0.0034	* 5.3191	-2.3937	1.0533	-0.6445	0.0042	0.0042	0.0042	0.0042	
MN CL	2	3.7000	10.1435	-1.0149	1.6196	-3.2245	1.9546	0.0020	* 6.0719	-1.9478	0.1092	0.0020	0.0020	0.0020	0.0020	
FE CL	1	11.0006	-1.1059	0.7944	-1.5902	G.8381	0.0115	* 5.8588	-2.0851	0.2137	0.0027	0.0027	0.0027	0.0027	0.0027	
CU CL	8	3.9300	10.4843	-0.6643	0.3641	0.992	-C.9416	0.0023	* 5.3337	-2.3772	1.3426	-1.7651	0.9722	0.0015	0.0015	
ZN CL	1	2.1000	9.8821	-0.5316	-0.1242	-0.1776	0.0034	* 5.5624	-2.0868	0.2152	0.0007	0.0007	0.0007	0.0007	0.0007	
GA CL	3	4.9200	10.7355	-0.5423	-0.5943	0.0406	0.0034	* 5.4456	-2.2371	0.6892	-0.4290	0.0043	0.0043	0.0043	0.0043	
GE CL	4	4.4000	10.4551	-0.8067	-0.3883	0.0039	* 5.9048	-2.1668	0.0789	0.0021	0.0021	0.0021	0.0021	0.0021	0.0021	
AS CL	1	10.3224	-0.8430	0.3762	-0.4350	0.014	* 5.8119	-2.0622	0.2286	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	
SE CL	2	10.7188	-0.9488	-0.1355	0.0104	* 5.6489	-1.9190	0.1611	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	0.0029	
BR CL	1	2.2330	10.7561	-0.1150	-1.4691	C.6463	0.3717	0.0063	* 5.4070	-2.6142	1.3952	-0.4960	0.0052	0.0052	0.0052	
RB CL	1	4.3400	9.9064	-0.7199	1.6024	-3.5467	2.1773	0.0027	* 5.9489	-2.3042	0.1268	0.2416	0.0013	0.0013	0.0013	
SR CL	4	4.1600	9.8012	-1.2949	2.3444	-3.0177	1.5467	0.0038	* 5.8139	-2.2787	0.7514	-0.4649	0.0031	0.0031	0.0031	
Y CL	2	11.0660	-1.2883	1.0142	-0.6058	-0.4550	0.0049	* 5.5251	-2.2064	0.6068	-0.3387	0.0028	0.0028	0.0028		
AG CL	2	3.2200	10.2885	-0.3907	-0.3742	0.0038	* 5.5561	-2.1961	0.4940	0.1860	0.0013	0.0013	0.0013	0.0013		
CD CL	1	2.1200	9.8054	-0.5097	-0.2603	0.0009	* 5.7504	-2.0634	0.1905	0.0010	0.0010	0.0010	0.0010	0.0010		
IN CL	3	4.4400	10.5285	-0.6450	-1.0931	0.7648	0.013 *	* 5.6456	-2.2800	0.7400	-0.4681	0.0042	0.0042	0.0042		
SN CL	3	10.2282	-0.9403	-0.8195	0.3564	0.013 *	* 6.0510	-2.3946	0.2987	0.0030	0.0030	0.0030	0.0030	0.0030		
SB CL	2	10.3567	-0.8450	0.6204	-0.2841	0.035 *	* 5.8864	-2.1332	-0.663	0.0012	0.0012	0.0012	0.0012	0.0012		
TE CL	1	10.2457	-0.9424	0.0756	-5.5104	-5.2217	0.0031 *	* 6.1126	-1.9473	0.1101	0.0021	0.0021	0.0021	0.0021		
I CL	3	2.1531	10.5319	0.3459	-1.6943	-2.0504	0.0018 *	* 5.6694	-2.2958	1.3958	0.8768	-1.7474	0.0084	0.0084		

TABLE 5—Continued

MOL.	N	DO	EQUILIBRIUM CONSTANT					PARTITION FUNCTION								
			STATES	B0	B1	B2	B3	B4	B5	MAX. ER.*	*	A0	A1	A2	A3	A4
CS CL	1	4.5800	9.9334	-1.1912	2.8233	-3.8854	-0.5854	2.7110	0.0047 *	6.0479	-2.3133	0.2312	0.1311	0.0048		
BA CL	10	4.5500	9.9594	-1.1995	0.9232	2.02392	-2.6158	0.0054 *	6.0299	-2.5102	1.0500	-0.5580	0.0031			
YB CL	3		9.6866	-1.0826	3.0713	-6.6055	4.3000	0.0053 *	5.9687	-2.1767	0.2766	0.0029	0.0029			
AU CL	1	3.5000	10.4491	-0.9692	0.4074	-0.2975		0.0038 *	5.5640	-2.0523	0.2002	C.0008				
HG CL	1	1.0400	9.6012	-0.4731	-0.0125	-0.2918		0.0038 *	6.0249	-2.1049	-0.0366	0.2703	0.0031			
TL CL	2	3.8200	10.2434	-0.7136	-0.0901	0.0752		0.0039 *	5.7692	-2.2558	0.4817	-0.2245	0.0013			
PB CL	3	3.1000	9.8253	-1.2422	0.4309	0.9152	-1.2224	0.0025 *	5.9996	-2.2534	0.4921	-0.1698	0.0010			
AL SE	2	3.4600	10.7857	-0.7858	-0.1407			0.0027 *	5.4873	-2.0722	0.2604	D.0024				
SI SE	1	5.6400	11.3895	-0.9755	-0.0901			0.0023 *	5.01075	-2.0100	0.2322	0.0011				
CU SE	3	2.5500	10.0783	-0.9668	0.9568	-0.6674		0.0028 *	6.01556	-2.3030	0.1452	0.0023				
GE SE	1	4.9800	11.2384	-1.1163	0.3775			0.0015 *	5.5644	-2.0873	0.2463	0.0023				
K BR	1	3.9100	9.7968	-0.7823	1.8098	-3.8842	2.5552	0.0031 *	6.0128	-2.3146	0.1345.	0.2360	0.0053			
SI TE	1	4.6400	11.1445	-1.0274	0.2402	-0.1432		0.0036 *	5.3406	-1.9922	0.1831	0.0013				
GE TE	1	4.2400	11.0317	-1.1431	-0.1381	-0.5358		0.0039 *	5.8258	-2.0101	0.2184	0.0027				
K I	1	3.3100	9.6625	-0.7210	1.8703	-3.9239	2.5006	0.0028 *	6.1888	-2.3327	0.1594	0.0052				
H H	1	4.4781	11.1759	-0.8735	-0.7470	0.7478		0.0007 *	1.6498	-1.6265	0.7472	-0.2751	0.0007			
H H +	1	2.6508	9.9835	-0.0664	-1.4979	-0.0195	0.7486	0.0054 *	2.5410	-2.4336	1.4979	0.0192	-0.7483	0.0054		
HE HE +	1	2.3650	10.2190	-0.4011	-0.6310			0.0029 *	3.2041	-2.0411	0.8289	0.6310	0.0029			
LI LI	4	1.0460	9.4736	-0.3274	1.1962	-3.5541	2.4491	0.0030 *	4.6515	-2.0580	0.4341	0.0016				
B B	2	3.0200	11.0585	-0.4932	-0.3893			0.0020 *	4.2793	-2.0492	0.4345	0.0029				
C C	8	6.2100	11.4576	-0.4458	-0.1818			0.0026 *	4.3091	-2.2406	0.4865	-0.2049	0.0012			
C C +	1	5.3200	11.4535	-0.7842	-0.0300	-0.3124		0.0004 *	5.3200	-1.8188	0.2984					
N N	1	9.7594	11.8838	-0.8915	0.2929	-1.4224	0.9007	0.0009 *	3.2643	-1.7303	0.4192	0.0025				
N N +	4	8.7128	11.8072	-0.4420	-0.5843	-0.9278	0.8821	0.0018 *	3.6830	-2.1583	0.9929	-0.2181	0.0031			
O O	6	5.1156	11.8558	-0.5309	-0.6214			0.0011 *	4.0636	-2.0779	0.7660	-0.2111	0.0016			
O O +	2	6.6630	11.5549	-0.7335	-0.3005	-0.1753		0.0007 *	4.194	-1.8480	0.4661	0.0027				
F F	1	1.6020	11.6249	-0.3917	-0.5115	-0.1205		0.0027 *	4.0355	-2.1726	0.4608	0.0036				
NE NE +	1	1.3000	10.2518	-0.6359	-0.103			0.0027 *	4.6665	-1.9305	0.1411	0.0026				
NA NA	4	0.7200	9.2096	-0.1176	1.1635	-5.6561	8.6389	-4.7450	0.0020 *	5.6752	-2.6810	0.6626	-0.1283	0.0020		
MG MG	2	0.0501	8.6463	-1.6726	1.6431	-3.332	2.4266	0.0044 *	5.6533	-1.0891	0.1211	-0.854	0.0008			
AL AL	2	1.5500	10.3474	-0.2335	-0.2761	-0.7144	0.6243	0.0018 *	5.5538	-2.3365	0.5754	-0.2119	0.0011			
SI SI	3	3.2100	11.0799	-0.7830	-0.5694	0.8076	-0.8107	0.0009 *	5.2617	-2.1485	0.5647	-0.2285	0.0037			
P P	4	5.0330	11.2490	-0.9821	0.2367	0.8887	-1.3142	0.0050 *	4.9884	-2.1415	1.1375	-1.8111	1.2663			
P P +	6	4.9900	10.7616	-0.8035	0.322	0.0919	-0.7295	0.0028 *	5.2762	-2.2351	0.4167	-0.1852	0.0039			
S S	2	4.3693	11.2917	-0.6065	-0.1125	-0.3562		0.0016 *	5.0796	-2.1967	0.4101	0.0030				
S S +	1	5.3700	10.9811	-0.9318	0.4197	-0.6452		0.0019 *	5.0598	-1.8928	0.2034	0.0034				
CL CL	1	2.4794	11.2793	-0.5356	-0.4665			0.0032 *	4.7438	-2.1109	0.3280	0.0033				
K K	4	0.5140	8.9949	-1.1018	3.043	-6.1302	3.2656	0.0037 *	6.2963	-2.3873	0.2118	0.0041				
CU CU	3	2.0300	10.1749	-0.9712	1.1405	-0.8963	0.040	0.0040 *	5.4806	-2.4706	0.8867	-0.4736	0.0018			
AS AS	5	3.9600	11.0864	-0.7253	-0.2214	1.2887	-1.1896	0.0025 *	5.2506	-2.4520	1.5981	-1.9349	0.9330	0.0023		
SE SE	2	11.0950	-0.9844	0.0343	0.2123			0.0006 *	5.7320	-2.1070	0.0029					
SB SB	1	3.0900	11.0023	-1.2817	1.014	0.0551	-0.7954	0.0032 *	5.7012	-2.0571	0.1630	0.0012				
TE TE	2	2.6770	10.7951	-0.7579	0.4198	0.9161	-1.1418	0.0006 *	6.1915	-2.4514	0.164	0.1181	0.0035			
I I	1	1.5424	10.6380	-0.4931	-0.0491			0.0027 *	5.9902	-2.2284	0.2711	0.0028				

$^3\Sigma^-$. If the temperature is low enough that we can neglect excited states, we have, therefore,

$$\frac{Q(\text{CH}^-)}{Q(\text{CH})} \approx \frac{g_e(\text{CH}^-)}{g_e(\text{CH})} = \frac{g_e(^3\Sigma)}{g_e(^2\Pi)} = \frac{3}{4},$$

because $g_e = (2 - \delta_{0,\Lambda})(2S + 1)$. This ratio is almost independent of temperature.

IV. ORGANIZATION OF THE TABLES

a) Tables of Coefficients for Molecular Partition Functions and Equilibrium Constants

Table 5 gives the coefficients a_n of the following polynomial development in $\log Q$, and the coefficients b_n of the following development in $\log {}^pK$ in the temperature range 1000–9000 K:

$$\log Q = \sum_{n=0}^{n'_{\max}} a_n (\log \theta)^n \quad (16)$$

$$\log {}^pK = \sum_{n=0}^{n''_{\max}} b_n (\log \theta)^n - \theta D_0^0. \quad (17)$$

The total number of coefficients relative to $\log Q$, n'_{\max} , which ranges between 2 and 5, depends on the accuracy of the fitting polynomial; the number of coefficients relative to $\log {}^pK$, n''_{\max} , is always less than or equal to 6. Table 5 also gives the maximum error obtained from these expansions, for both $\log Q$ and $\log {}^pK$; it is generally much smaller than 0.01 dex for the fit alone. This error does not take account of errors that may arise from the adopted spectroscopic constants themselves and from the molecular model given in equation (1). An error in D_0^0 can be easily corrected through equation (17), but other errors are much more difficult to estimate. The neglect of low-lying electronic states or a wrong multiplicity or an incorrect excitation energy may lead to large errors in Q . On the other hand, the effect of the model in the calculations of the partition function remains small in our temperature domain and is maximum at 9000 K.

For positive ions, the molecular formula is always printed as $A B^+$; as explained in § III, the dissociation products are A^+ and B , with $I(A) < I(B)$.

In these tables, $\theta = 5040/T$, where T is the temperature in kelvins, D_0^0 is in electron volts (nothing is printed when Huber and Herzberg 1979 give no D_0^0 value), and the equilibrium constant pK is in SI units (i.e., pascals or $N \cdot m^{-2}$). To convert to dyne cm^{-2} , add 1 to $\log {}^pK$. Table 5 also gives the number of electronic substates considered in the calculation of Q . For example, we count $^2\Delta$ as two substates, because, if the coupling is according to Hund's case a , the two substates will have different excitation energies, and this difference will be significant if the state is the ground or a low lying state. Electronic states up to 40,000 cm^{-1} have been generally accounted for; for some of our selected molecules, spectroscopic constants, designation of the ground state, or both, are badly or not known; in that case, only the ground electronic state has been included, and it appeared necessary to estimate one of the constants (ω_e , B_e , or g_e).

Table 5 is grouped in order of increasing atomic number of the lower Z of the two atoms in the molecule, then in order of increasing atomic number of the higher Z atom. Within each group, neutral atoms precede positive ions. We note that the

TABLE 6
NEUTRALIZATION ENERGIES $I(AB^-)$, DISSOCIATION ENERGIES D_0^0 , AND COEFFICIENTS q_n FOR
PARTITION FUNCTIONS OF NEGATIVE MOLECULAR IONS
 $\log_{10} Q(AB^-) = \sum_{n=0} q_n (\log_{10} \theta)^n, \theta = 5040/T$

Negative Ion	Neutralization Energy (eV)	Dissociation Energy (eV)	$\frac{g_e(AB^-)}{g_e(AB)}$		q_0	q_1	q_2	q_3	q_4
			$g_e(AB^-)$	$g_e(AB)$					
H ₂ ⁻	-3.	+0.73	2/1	+1.9508	-1.6265	+0.7472	-0.2751	...	
OH ⁻	+1.83	+4.76	1/4	+2.4908	-1.6778	+0.6743	-0.1874	...	
CN ⁻	+3.82	+10.31	1/2	+3.7068	-2.1514	+0.9226	-0.1671	...	
C ₂ ⁻	+3.54	+8.48	2/1	+4.6101	-2.2406	+0.4865	-0.2049	...	
SiH ⁻	+1.28	+3.23	3/4	+3.5659	-1.9801	+0.7704	-0.2247	...	
HS ⁻	+2.32	+3.79	1/4	+2.8914	-1.8385	+0.5852	
CS ⁻	+1.2	+6.5	4/1	+4.7667	-1.9348	+0.8034	-1.3669	+1.1561	

TABLE 7
COEFFICIENTS FOR ATOMIC PARTITION FUNCTIONS

ELEMENT	PARTITION FUNCTION				PARTITION FUNCTION								
	MAX.E.	CO	C1	C2	C3	C4	ELEMENT	MAX.E.	CO	C1	C2	C3	C4
H	0.00000	0.30103	-0.00000				BR+	0.00254	0.82697	-0.30362	0.17411		
H +	0.00000	0.00000	0.00000				PB	0.00238	0.35159	-0.50067	1.74930	-2.50288	1.24577
HE	0.00000	0.00000	0.00000				SR	0.00497	0.10160	-0.98646	3.21529	-4.18242	1.84624
HE +	0.00000	0.30103	0.00000				Y	0.00543	0.0078	1.07403	-0.90007	1.32443	
L1	0.00128	0.31804	-0.20616	0.91456	-1.66121	1.04159	ZR	0.00078	1.51403	1.10749	0.71584	-0.30517	
BE	0.00619	0.00801	-0.17135	0.62921	-0.58945		NB	0.00093	1.72193	-0.96931	0.84701	-0.77242	
BE +	0.00289	-0.30389	-0.00819				RU	0.00259	1.53544	-0.95790	0.65520	-0.19002	
B	0.00319	0.78028	-0.01622				RH	0.00403	1.42445	-0.73816	0.28160		
B +	0.00377	0.00349	-0.01035				PD	0.00548	1.46119	-1.51528	0.26006	2.97576	-2.29501
C	0.00375	0.96752	-0.09452	0.08055			AG	0.00379	0.30188	-0.01088			
C +	0.00284	0.77239	-0.02540				CD	0.00000	0.00000	0.00000			
N	0.00279	0.60683	0.08674	0.30565	-0.28114		IN	0.00262	0.61694	-0.35160	-0.28054	0.29267	
N +	0.00362	0.94968	-0.06463	-0.01291			SN	0.00342	0.71534	-0.76319	0.494970	0.44099	
O	0.00325	0.95033	-0.05703				SB	0.00314	0.67754	-0.39920	0.64590	-0.31914	
O +	0.00037	0.60405	-0.03025	0.04525			TE	0.00203	0.79722	-0.32317	0.26550		
F	0.00072	0.76284	-0.03582	-0.05619			I	0.00191	0.62132	-0.10197	0.10197		
NE	0.00000	0.00000	0.00000				CS	0.00710	0.40691	0.66458	2.87484	-3.24127	1.10631
NE +	0.00033	0.74847	-0.06562	-0.07088			BA	0.00534	0.40430	-1.93697	2.13107	1.56992	-2.64798
NA	0.00328	0.30955	-0.17778	1.10594	-2.42847	1.70721	LA	0.00302	1.43627	-1.44018	0.81057	-0.23872	
MG	0.00239	0.00556	-0.12840	0.81506	-1.79635	1.26292	CE	0.00170	2.28110	-1.87712	0.23104	0.45862	
MG +	0.00164	0.30257	-0.00451				TB	0.00302	2.22568	-1.38227	0.91401	-0.22808	
AL	0.00268	0.76786	-0.05207	0.14713	-0.21376		HO	0.00813	1.54615	-1.77233	2.45212	0.48439	-1.98287
AL +	0.00365	0.00334	-0.00995				YB	0.00512	0.04191	0.69224	3.49819	-6.64720	4.20480
SI	0.00318	0.97896	-0.19208	0.04753			LU	0.00231	0.94528	-0.67678	0.02821	-2.06203	1.54988
SI +	0.00199	0.75647	-0.05490	-0.10126			HF	0.00337	1.16596	-1.11790	0.69486		
P	0.00179	0.64618	-0.31132	0.68633	-0.47505		TA	0.00266	1.23359	-1.44778	0.84884		
P +	0.00094	0.93588	-0.18848	0.08921	-0.22447		TA +	0.00081	1.36331	1.29035	0.13472	0.34727	
S	0.00376	0.95254	-0.15166	0.2340			W	0.00348	1.11208	-1.41233	0.27987	-1.21831	1.28689
S +	0.00251	0.61971	-0.17465	0.48283	-0.39157		IR	0.00349	1.31959	-0.83851	0.55564		
CL	0.00041	0.74465	-0.07389	-0.06965			PT	0.00057	1.29156	-0.34013	0.17630	-0.25884	
CL +	0.00339	0.92728	-0.15913	-0.01983			AU	0.00381	0.38900	-0.44824	0.68902	-0.31529	
K	0.00209	0.34419	-0.48157	1.92563	-3.17821	1.83211	HG	0.00132	0.00120	-0.00360			
CA	0.00388	0.07460	-0.75759	2.58494	-3.53170	1.65240	HG +	0.00168	0.30562	-0.00465			
SC	0.000581	1.08209	-0.77814	1.78504	-1.39179		TL	0.00325	0.38523	-0.36653	0.45713	-0.14146	
TI	0.00244	1.47343	-0.97220	1.47986	-0.93275		PB	0.00302	0.19574	-0.92697	0.99476	0.82393	-1.33084
V	0.00434	1.68359	-0.82055	0.92361	-0.78342		BI	0.00173	0.62814	-0.50277	0.37664		
CR	0.000449	1.02332	-1.02540	0.202181	-1.32723		TH	0.00633	1.42677	-1.89720	1.03185	0.33964	
MN	0.00201	0.80810	-0.39108	1.74756	-3.13517	1.93514	U	0.00299	1.92666	-2.05483	0.90354	2.82611	-2.77207
FE	0.00382	1.44701	-0.67040	1.01267	-0.81428								
CO	0.00436	1.52929	-0.71430	0.37210	-0.23278								
NI	0.00392	1.49063	-0.33662	0.08553	-0.19277								
CU	0.00209	0.36884	-0.46740	1.02157	-0.70872								
ZN	0.00024	-0.00147	-0.02804	0.16255	-0.17855								
ZN +	0.00024	0.30123	-0.00062										
GA	0.00466	0.71314	-0.21023	0.14158	-0.37944								
GE	0.00420	0.88280	-0.40360	-0.23805									
AS	0.00197	0.65368	-0.33297	0.67256	-0.42734								
AS +	0.00282	0.77362	-0.56486	-0.26137									
SE	0.00198	0.87375	-0.29536	0.09633									
BR	0.00322	0.66881	-0.15099	0.07533									

coefficient a_1 in the expansion for $\log Q$ is in most cases close to -2 , and that, provided the expansion is terminated at a_3 , the coefficients usually satisfy $|a_0| > |a_1| > |a_2| > |a_3|$. In the expansion for $\log^p K$, the coefficients b_1 to b_5 are roughly of the same magnitude.

In a conversation with J. B. T., Dr. Alan Irwin has pointed out that the approximation to the partition function calculated for a particular temperature from its polynomial expansion may not be consistent with the approximation to the equilibrium constant calculated for the same temperature calculated from its polynomial expansion. Irwin has expressed the view that it would be preferable for a reader to use the polynomial expansion to calculate Q , but he should then, in order to maintain consistency, calculate the corresponding K from the exact (and relatively simple) equation. We agree with Irwin in principle, but we believe that in any real astrophysical context the difference between the two procedures is quite negligible and that it is perfectly safe to use the polynomial expansions for Q and K simultaneously. The reader who has doubts is, of course, free to follow Irwin's suggestion if he so wishes.

The most severe source of error in the partition function is the possibility of an unknown, or incorrectly placed, or incorrectly designated low-lying electronic state of high multiplicity. For example, if the term value of a state were changed from 2000 to 4000 cm^{-1} , $\log Q$ for that state would change by a factor of $\sim 0.25\theta$, where $\theta = 5040/T$. An additional source of error in the equilibrium constant is the uncertainty in D_0^0 ; if this uncertainty is ΔD_0^0 eV, the resulting uncertainty in $\log^p K$ is $\theta \Delta D_0^0$, which may be severe at low temperatures. Should a revised D_0^0 appear in the literature, however, the correction is easily made, although we stress again that it might be counterproductive to change pK for every new published value of D_0^0 , unless the previous value is shown to be quite definitely wrong.

If, following Shankar and Littleton (1983), we use Murad and Hildenbrand's (1975) value of $D_0^0 = 7.89$ eV for ZrO , we obtain excellent agreement (better than 0.06%) with Shankar and Littleton's five-parameter expansion in T for $\ln K$, but at 8000 K (where ZrO is hardly significant) our results differ from those of Shankar and Littleton by 6%.

b) Table of Coefficients of Partition Functions of Negative Molecular Ions

The expansion we have chosen in the temperature range 1000–9000 K is

$$\log Q = \sum_{n=0}^4 q_n (\log \theta)^n. \quad (18)$$

Table 6 gives the coefficients q_n for seven negative molecular ions of astrophysical interest.

For reasons explained in § III, we have not tabulated equilibrium constants for negative molecular ions. Instead, in Table 6 we also list the dissociation energies $D_0^0(AB^-)$ and neutralization energies $I(AB^-)$.

c) Table of Coefficients of Atomic Partition Functions

Table 7 gives the coefficients c_n of the following series development of $\log Q$ for all neutral and singly ionized atoms represented in the molecules of Table 5:

$$\log Q = \sum_{n=0}^{n_{\max}} c_n (\log \theta)^n. \quad (19)$$

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