

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

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Received 1983 November 21; accepted 1984 March 29

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 artifices 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 the 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 even 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 are 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 all 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

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. Hefferlin 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:

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

We must note that higher order correction constants are seldom known for the selected molecules. Moreover, even first-order terms ($\alpha_e, \omega_e x_e$) 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.

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_0^0 , unobserved states, g_e, T_e , etc.).

It is interesting to consider an example to investigate how Q , the partition function, varies with temperature, for example, in the case of H₂ 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 1000–9000 K a good fit might be obtained from a polynomial in $\log T$ or in $\log \theta$, where $\theta = 5040/T$.

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

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

TABLE 1
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 0.3ω	1
$0.5B$ – $3.7B$	J summation	0.3ω – 1.2ω	v summation
Above $3.7B$	$\frac{kT}{hcB} + \frac{1}{3}$	above 1.2ω	$\frac{kT}{hc\omega} \times 10^{0.29\omega/T}$

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

^b ω is the vibrational constant in cm^{-1} .

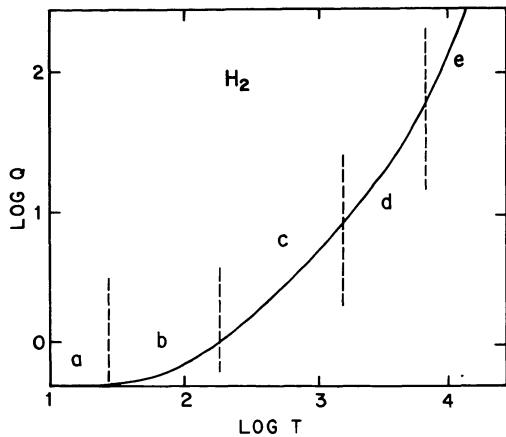


FIG. 1.

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 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

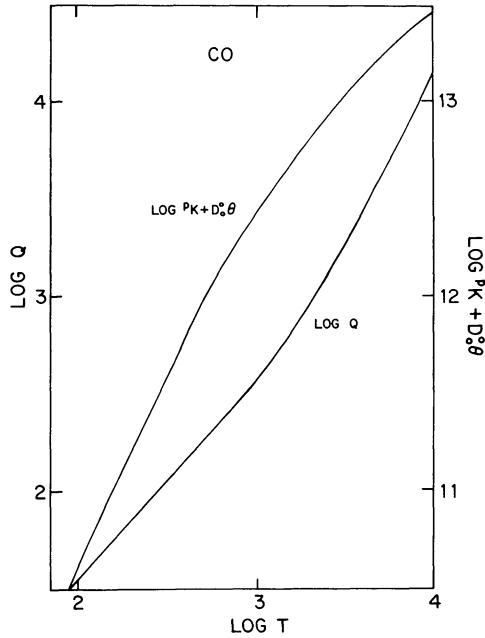


FIG. 2

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	$500 < T < 6000$	$\log Q(\text{CO}) = 3.095 + 0.02262\theta - 0.000682\theta^2 - 1.059\Lambda + 0.72133/\theta - 0.27823/\theta^2 + 0.05547/\theta^3$
	$1000 < T < 20,000$	$\log Q(\text{CO}) = 4.088 + 0.4028\theta - 0.01859\theta^2 - 4.0697\Lambda - 1.08196/\theta + 0.24836/\theta^2 - 0.01947/\theta^3$
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 $Q(\text{Fe})^{\text{a}}$

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	$1000 < T < 16000$	$\ln Q = -1156.095 + 746.598l - 192.8657l^2 + 24.966l^3 - 1.6193l^4 + 0.042118l^5$
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 $\log^p K (\text{CO})^{\text{a}}$

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 pK was in atmospheres, and in Kurucz (1970) $\log(1/{}^pK)$ 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:

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

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

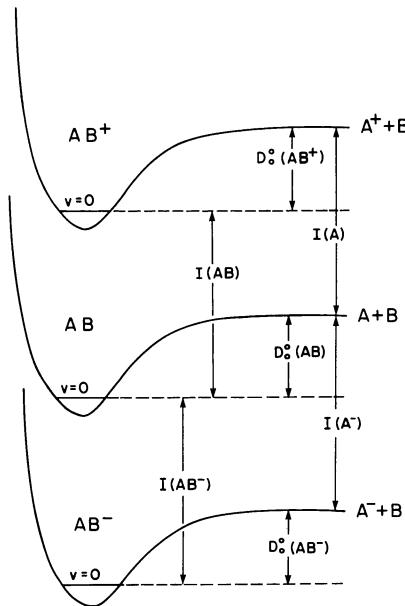


FIG. 3.—Illustrating the relations $D_0^0(AB^-) + I(A^-) = D_0^0(AB) + I(AB^-)$, $D_0^0(AB) + I(A) = D_0^0(AB^+) + I(AB)$. Potential curves are relative to the ground states of AB , AB^+ , and AB^- .

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 $(\log \theta K + \theta D_0^0)$ 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	STATES	EQUILIBRIUM CONSTANT					PARTITION FUNCTION					MAX. ER.			
			D ₀ (EV)	B ₀	B ₁	B ₂	B ₃	B ₄	B ₅	A ₀	A ₁	A ₂	A ₃	A ₄		
L	H	1	2.4287	9.9506	-0.5163	0.1813	-1.7211	1.2805		0.0031*	3.2564	-2.1799	0.7236	-0.1052	0.0026	
BE	H	3	2.0340	9.6644	-0.6592	-0.2541	-0.2677		0.0033*	3.2507	-2.0115	0.8852	-0.3253	0.0030		
B	H	5	3.4200	10.5064	0.1929	-0.3299	-1.4246	0.6362		0.0034*	3.1862	-2.6821	0.5142	0.6959	0.0056	
C	H	5	3.4650	10.5263	-0.5284	-0.7239				0.0027*	3.3586	-0.6056	0.9624	-0.2339	0.0008	
N	H	4	3.4700	10.4609	-0.7387	-0.5713				0.0034*	3.0735	-1.8501	0.9607	-0.3935	0.0019	
O	H	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				0.0040*	2.4164	-1.6132	0.6357	-0.1767	0.0008	
NA	H	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	H	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	
AL	H	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	
SI	H	2	3.0600	10.2379	-0.7143	-0.6404	0.1156			0.0031*	3.6908	-1.9801	0.7704	-0.2247	0.0021	
P	H	4	3.0200	10.1061	-0.7236	-0.2853	-0.2032			0.0014*	3.4957	-2.0871	0.9617	-0.2598	0.0007	
S	H	3	3.5500	10.4445	-0.8190	-0.5524				0.0014*	3.4935	-1.8385	0.5852	0.0036		
H	CL	1	4.4336	10.9013	-0.8274	-0.5974				0.0025*	2.8005	-2.025*	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	0.0051	
CA	H	9	1.7000	9.1952	-0.8802	1.1610	-2.5221	1.3514		0.0015*	3.8411	-2.3891	1.3578	-0.6893	0.0042	
CR	H	2	2.5000	9.8837	-1.2266	1.1519	-1.9385	0.9790		0.0025*	4.0929	-2.2491	0.8923	-0.1787	0.0031	
MN	H	2	CO	H	2	9.5870	-0.7116	0.8607	-2.8120	1.8726	0.0026*	4.1860	-2.1839	0.8747	-0.2513	0.0016
CO	H	2	CO	H	2	10.3877	-0.8742	1.4621	1.4621		0.0022*	4.1047	-2.6262	0.4803	0.2721	0.0060
NI	H	4	3.0700	10.7821	-0.4987	-1.0040	0.3197			0.0037*	3.6736	-2.3271	1.0818	-0.5336	0.0037	
CU	H	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	
ZN	H	4	0.8510	9.3436	-0.3528	-0.0866	-1.2327	0.8192		0.0005*	3.6197	-2.1349	0.3017	0.3458	0.0035	
GA	H	3	2.8400	10.3733	-0.3071	-1.3737	0.0238	0.5134		0.0055*	3.3100	-2.3703	1.4724	-0.7575	0.0046	
GE	H	2	3.0000	10.0536	-0.8571	-0.8573			0.0013*	3.7954	-2.0472	0.6234	0.0036			
AS	H	1	3.6000	10.1156	-1.1074	0.3885	-0.5746		0.0013*	3.5022	-1.7207	0.3759	0.0036			
SE	H	1	3.2000	10.2854	-1.1036	-0.3013			0.0017*	3.5571	-1.6887	0.3912	0.0031			
H	BR	1	3.7580	10.7059	-0.8545	-0.5918	0.1995		0.0012*	2.9356	-1.8051	0.5439	0.0023			
RB	H	2	9.4673	-0.6489	1.3539	-3.5418	2.2686		0.0026*	3.8516	-2.2990	0.4213	0.2106	0.0058		
SR	H	6	1.6600	9.1300	-1.0867	1.9505	-3.5983	1.8586	0.0025*	3.9406	-2.3979	1.2564	-0.5865	0.0029		
PD	H	1	10.0979	-2.2770	-0.0175	2.7905	-2.2384		0.0054*	3.3378	-1.7316	0.3697	0.0037			
AG	H	6	2.2800	10.0411	-0.4123	-0.7461	0.1382		0.0015*	3.2301	-2.0994	0.8105	-0.2140	0.0011		
CD	H	4	0.6780	9.2759	-0.4191	-0.6388	0.1624		0.0029*	3.6946	-2.0809	0.6389	-0.1625	0.0030		
IN	H	4	2.4800	10.1447	-0.3957	-1.7087	0.5557	0.5123	0.0044*	3.4418	-2.4303	1.4516	-0.6835	0.0047		
SN	H	1	2.7300	9.8505	-1.4863	-0.6936	0.2966		0.0036*	3.8521	-1.7739	0.3402	0.0041			
SB	H	1	9.9235	-1.0973	0.4311	-0.4708			0.0032*	3.7208	-1.7994	0.3179	0.0037			
TE	H	1	10.0053	-1.0836	-0.0154	-0.1301			0.0017*	3.7592	-1.7365	0.3667	0.0028			
H	I	1	3.0541	10.4946	-0.7350	-0.4527			0.0025*	3.1038	-1.8753	0.5591	0.2409			
1	8.1000	9.4674	-1.1765	2.7899	-4.0266	-0.5222	2.6745		0.0048*	3.9070	-2.2534	0.3373	0.0052			
BA	H	9	1.9500	9.2562	-0.9602	-1.9128	2.8211	3.7826	-6.1227	0.0101*	4.1275	-3.4447	3.4772	-1.6164	-0.6508	
LA	H	1	10.5707	-2.0868	0.6501	-0.3842			0.0029	3.8330	-1.8516	0.2606	0.0128			
YB	H	5	1.9300	9.1165	-0.8337	2.3885	-6.1903	4.1950		0.0063*	3.8992	-2.3567	1.0469	-0.3525	0.0029	
LU	H	1	10.5132	-1.1430	0.3964	-1.8500	1.4373		0.0026*	3.4069	-2.0439	0.5556	0.0035			
PT	H	6	3.4400	10.5855	-0.8305	-0.9753	0.7861	-0.6278	0.0012*	3.6862	-2.0426	1.1143	-0.5023	0.0045		
AU	H	2	3.2200	10.3037	-1.0665	-0.0737	0.4760	-0.7257		0.0023*	3.0567	-1.9182	0.7472	-0.2103	0.0020	
HG	H	3	0.3744	9.2284	-0.5946	0.1954	-0.5625			0.0021*	3.7548	-1.9107	0.1771	0.5661	0.0020	
TL	H	1	1.9700	9.8718	-0.4509	-0.8717	0.5256	-0.0995		0.0042*	3.4880	-2.4274	1.2776	-0.8665	0.0054	
PB	H	3	1.5900	9.1386	-0.9871	-0.4793	1.3671	-1.1166		0.0040*	4.0319	-2.4374	1.4150	-0.5829	0.0058	
BI	H	3	2.9000	9.6707	-0.2999	-0.2473	-1.0153	0.6873		0.0004*	3.9292	-2.3670	0.8067	0.0038		
HE	H	+	1	1.8450	10.1667	-0.4814	-0.6444	-0.7916	0.8534	0.0015*	2.3613	-1.9733	0.6761	0.0794	0.0060	
BE	H	+	2	3.1400	9.7188	-0.7267	0.0041	-1.0889	0.7404	0.0010*	2.8969	-1.9119	0.5829	0.0036		

TABLE 5—Continued

MOL.	N STATES	EQUILIBRIUM CONSTANT						PARTITION FUNCTION						MAX. ER.	
		D0 (EV)	B0	B1	B2	B3	B4	B5	A0	A1	A2	A3	A4		
B	H +	1.9500	10.3048	-0.7004	-0.5024				0.0005	*	3.0915	-1.8213	0.5252	0.0020	
C	H +	4.0850	10.7018	0.0994	-1.4610	-0.8279	1.3625		0.0035	*	2.8849	-2.6920	1.6342	0.0038	
N	H +	3.3900	9.6574	-0.6294	-0.6294	0.1927			0.0014	*	3.5792	-1.9573	0.9387	0.0040	
O	H +	5.0900	10.4950	-0.6799	-0.9224	0.3310			0.0029	*	3.0879	-1.8739	0.9959	0.0034	
H	F +	2.4320	10.6684	-0.6549	-0.9526	0.2645			0.0029	*	3.2093	-1.9027	0.9429	0.0012	
NE	H +	2.0800	10.1080	-0.8691	-0.4086				0.0022	*	2.5352	-1.6309	0.4086	0.0022	
MG	H +	2.0800	9.4108	-0.5435	0.0987	-1.7288	1.3461		0.0035	*	3.2458	-2.0802	0.6259	0.0039	
AL	H +	2.1700	10.5758	-0.7532	-0.8627	0.1410			0.0012	*	3.6272	-1.8270	0.3655	0.0031	
SI	H +	3.3600	9.7604	-1.1045	-0.3654	0.5871			0.0036	*	3.0519	-1.9409	-0.3415	0.0027	
P	H +	1.34800	10.2741	-0.9924	-0.2456	-0.2060			0.0022	*	3.5374	-1.7004	0.3861	0.0033	
S	H +	4.6530	10.4094	-0.8021	-0.6304				0.0009	*	3.3283	-1.6545	0.4028	0.0018	
ZN	H +	2.5000	9.5271	-0.4794	-0.5934				0.0025	*	3.4719	-1.8460	0.7283	0.0014	
H	BR +	3.6940	10.2047	-0.9225	-0.5992	0.2723			0.0043	*	3.1362	-2.0520	0.7530	0.0016	
CD	H +	2.1000	9.4122	-0.4222	-0.6361				0.0020	*	3.5928	-1.8837	0.7143	0.0016	
HG	H +	2.9930	9.5121	-0.5024	-0.6184				0.0037	*	3.2572	-2.0778	0.6361	0.0017	
C	N	7.7600	11.4479	-0.4840	-0.4160	-0.9435	0.8380		0.0036	*	3.1604	-2.0039	0.6274	0.0041	
C	O	11.0920	12.2263	-0.8829	-0.1230	-0.3226			0.0015	*	4.0078	-2.1514	0.9226	0.0033	
C	F	5.6700	11.1538	-0.6431	-0.4255				0.0011	*	3.6076	-1.7608	0.4172	0.0024	
SI	C	4.6400	10.8445	-0.9184	0.1532	-0.3771			0.0012	*	5.1477	-1.8671	0.2404	0.0037	
C	P	5.2800	11.0579	-0.4737	0.1729	-1.2021	C. 5631		0.0025	*	4.6258	-2.3994	0.7464	0.0044	
C	S	7.3550	11.8298	-0.8130	-0.5170	1.1553	-1.2249		0.0036	*	4.1646	-1.9348	0.8034	0.0030	
C	CL	5.9800	11.6323	-0.8887	-0.3397	0.3565			0.0015	*	5.0103	-2.0870	0.3565	0.0034	
C	SE	4.1100	10.5034	-0.8128	0.0167				0.0020	*	4.4060	-2.0380	0.6731	0.0053	
C	BR	4.0100	11.8689	-1.0481	-0.5630	0.3225			0.0033	*	5.3299	-1.9319	0.1366	0.0025	
RH	C	6.4500	11.6317	-1.0444	0.0162				0.0012	*	4.7382	-2.2834	0.9149	0.0014	
IR	C	6.2800	12.0345	-0.6227	-0.8549	0.2473			0.0042	*	4.9037	-2.3935	0.6410	0.0028	
PT	C	4.3500	12.0523	-0.3741	-0.6714	-0.7355	C. 6846		0.0034	*	4.4772	-2.3097	1.1982	0.0039	
C	N	3	8.3380	11.5907	-0.7647	-0.4319			0.0020	*	3.7429	-2.2451	0.9459	0.0043	
C	O	2	6.4968	11.2253	-0.8143	0.0446	-0.4529		0.0019	*	3.9001	-1.8498	0.6943	0.0029	
N	O	3	10.8500	10.9036	-0.5611	-0.4198			0.0018	*	4.5916	-1.9257	0.4475	0.0025	
N	F	3.5000	10.6045	-0.6697	-0.0703	-0.2794			0.0033	*	4.3073	-1.8255	0.3765	0.0019	
AL	N	2	10.1571	-0.5225	-0.1325	-0.2400			0.0038	*	4.5511	-2.0680	0.5972	0.0019	
SI	NN	6	11.0504	-0.4223	-0.4462	-0.2266			0.0021	*	5.3348	-2.1160	0.5845	0.0035	
P	N	2	6.3600	11.2316	-1.0111	0.6714	-0.8076		0.0042	*	4.6570	-2.3587	0.8819	0.0023	
N	S	5	4.8000	10.9036	-0.7786	0.0941	-0.3808		0.0029	*	4.1665	-1.8848	0.3521	0.0026	
N	CL	2	4.9000	11.7421	-1.7267	1.5855	-1.3639		0.0010	*	4.8052	-1.9619	0.3140	0.0019	
TI	N	1	4.9000	11.0571	-0.5225	-0.1325	-0.2400		0.0021	*	4.9171	-1.9905	0.3045	0.0020	
AS	N	1	11.1252	-0.9863	0.6970	-0.7720			0.0022	*	4.5568	-1.8253	0.2914	0.0041	
N	SE	6	4.0000	10.7173	-0.6078	-0.4482	0.3251		0.0022	*	4.4116	-1.9312	0.3194	0.0023	
ZR	N	1	5.8100	11.6496	-1.8280	0.8730	-0.7237		0.0033	*	5.0500	-2.2744	0.7939	0.0064	
NB	N	1	10.3506	11.6210	-0.8373	0.0676	-1.0507	0.6864		0.0020	*	4.7625	-1.8648	0.2434	0.0038
N	O	+	6.3000	11.2307	-0.8277	0.5112	-1.3707	0.7033		0.0022	*	5.2229	-1.8645	0.2439	0.0038
N	S	+	4.4900	10.0377	-0.4691	0.7661	-2.2854	1.3395		0.0007	*	3.5649	-1.7328	0.4241	0.0041
LJ	O	2	4.6000	10.6366	-0.5176	-0.4647	-3.7714	3.3677		0.0016	*	4.9296	-2.2751	0.2384	0.0016
BE	O	6	8.2800	11.6221	-0.7011	-0.4788			0.0045	*	4.1294	-3.1941	1.1968	0.0035	
E	O	4	2.2300	11.0588	-0.6355	-0.2688	-0.1683		0.0022	*	3.9953	-1.8665	0.5965	0.0033	
F	O	1	2.6000	10.0152	-0.8008	1.1032	-2.6609	1.7389		0.0007	*	4.7283	-1.9565	0.3311	0.0018
NA	O	1							0.0033	*	5.3711	-1.9284	0.1449	0.0026	

TABLE 5—Continued

MOL.	N	EQUILIBRIUM CONSTANT						PARTITION FUNCTION						MAX. ER.			
		D ₀ (EV)	B ₀	B ₁	B ₂	B ₃	B ₄	B ₅	A ₀	A ₁	A ₂	A ₃	A ₄				
M ₆	0	7	3.53300	9.7780	-0.0290	1.1725	-1.1724	0.0040	*	5.3182	-2.6502	-0.2781	-0.7823	1.3137	0.0016		
AL	0	6	5.27000	10.92653	0.0703	-0.2742	-1.4863	0.9291	0.0008	*	4.9191	-2.6291	0.5831	0.3163	0.0042		
S ₁	0	10	8.26000	11.8772	-0.8349	-0.5248	1.1271	-1.1984	0.0032	*	4.2275	-1.9144	0.7201	-1.3099	1.1657	0.0035	
P	0	4	6.15000	10.9860	0.9497	0.3972	-0.5660	0.0031	*	4.8326	-1.9182	0.3582	0.3582	0.0019	0.0019		
S	0	3	5.3590	11.3119	-0.5729	-0.3278	-0.2574	0.0011	*	4.7963	-2.1308	0.5224	0.5224	0.0014	0.0014		
CL	0	4	2.7505	10.8756	-0.5189	-0.3876	0.0025	*	5.0465	-2.1026	0.4208	-0.1725	0.0023	0.0023			
K	0	1	10.1915	-1.0847	1.9449	-3.4048	1.8810	0.0022	*	5.3500	-1.9476	0.1096	0.0020	0.0020			
CA	0	6	4.76000	10.2335	1.1684	1.8170	-6.3417	2.6646	1.9124	0.0060	*	5.0437	-3.4848	0.9872	-2.6956	0.0037	
SC	0	4	6.96000	11.5015	-1.1288	0.8607	-0.9294	0.0042	*	4.8065	-2.2129	0.9991	-0.5414	0.0046	0.0046		
TI	0	15	6.87000	11.4047	-1.1484	0.6478	-0.6737	0.0027	*	5.3051	-2.3739	0.8940	-0.3641	0.0020	0.0020		
V	0	4	6.41000	11.8610	-1.1543	0.0357	-0.4292	0.0021	*	5.0687	-2.2186	0.9545	-0.4592	0.0032	0.0032		
CR	0	2	4.40000	10.7452	-1.4464	1.4416	-1.1862	0.0025	*	5.5270	-2.1311	0.6523	-0.2533	0.0027	0.0027		
MN	0	2	3.70000	10.6819	-0.9413	1.3892	-2.9384	1.7034	0.0018	*	5.3855	-2.0226	0.3621	0.0038	0.0038		
FE	0	3	4.20000	11.1428	-1.3307	0.5711	-0.9041	0.0035	*	5.5642	-2.1947	0.5056	0.0012	0.0012			
N ₁	0	1	3.87000	11.8158	-0.9732	0.0667	-0.4076	0.0042	*	4.9367	-1.9163	0.1656	0.0029	0.0029			
CU	0	6	2.79000	10.2956	-0.7120	0.3346	-0.3684	0.0021	*	5.3500	-2.3114	0.7400	-0.4122	0.0026	0.0026		
GA	0	2	3.91000	11.0366	-0.6891	-0.0939	-1.1012	0.7611	0.0023	*	4.9645	-2.0340	0.3183	0.0067	0.0067		
GE	0	5	6.78000	11.6762	-0.912	-1.3023	1.3586	-1.2339	0.0026	*	4.4985	-2.0441	0.4119	-1.6102	1.2279	0.0023	
AS	0	6	4.98000	10.9016	-0.7982	0.4555	-0.5465	-0.0196	0.0024	*	5.0509	-2.1235	0.2440	0.0043	0.0043		
SE	0	7	4.41000	11.1518	-0.6351	-0.6997	0.4226	0.0027	*	5.0293	-2.2137	0.8127	-0.4546	0.0035	0.0035		
BR	0	3	2.3970	10.7396	-0.4693	-0.1983	0.0028	*	5.2352	-2.2395	0.2781	0.0025	0.0025	0.0025			
RB	0	1	10.1834	-1.1105	1.7616	-2.7337	1.2892	0.0024	*	5.4767	-1.9410	0.1221	0.0023	0.0023			
SR	0	6	4.88000	10.2479	-0.1106	1.8979	-6.3299	3.0605	1.5515	0.0066	*	5.1657	-2.1519	1.5631	1.8476	-2.3506	0.0040
Y	0	4	7.29000	11.4412	-1.3967	1.1101	-0.6405	-0.5930	0.0053	*	4.9515	-2.0866	0.6556	-0.3082	0.0038	0.0038	
ZR	0	17	7.85000	11.5031	-1.1916	0.5692	-0.1795	0.0039	*	5.3279	-2.4694	0.2164	-0.2313	0.0027	0.0027		
NB	0	1	7.80000	11.9070	-1.5994	0.6954	-0.9700	0.0011	*	5.1386	-1.9248	0.2897	0.0023	0.0023			
RU	0	1	5.30000	11.4963	-1.6269	0.6020	-0.4302	0.0024	*	5.3642	-1.8834	0.2173	0.0036	0.0036			
AG	0	6	2.29000	9.9937	-0.2994	-0.3504	0.0037	*	5.6400	-2.0866	0.4857	-0.1403	0.0020	0.0020			
IN	0	1	2.94000	10.8195	-0.2163	-0.4423	0.01520	0.0024	*	5.1354	-1.9915	0.2609	0.0013	0.0013			
SN	0	4	5.49000	11.3457	-1.2465	-0.9836	0.6380	0.0028	*	4.7103	-2.0718	0.6368	-0.3377	0.0055	0.0055		
SB	0	5	4.39000	10.8248	-0.6968	0.2752	0.4120	-0.9811	0.0025	*	5.1963	-2.3071	0.4144	-0.3374	0.0048	0.0048	
TE	0	2	3.90000	10.8627	-0.7738	0.0668	0.0039	*	5.2844	-2.1005	0.1946	0.0023	0.0023				
I	0	3	1.80000	10.6616	-0.2700	-0.2107	-0.1462	0.0037	*	5.3109	-2.3921	0.4198	0.0036	0.0036			
BA	0	7	5.79000	10.8582	-1.8538	-0.700	-0.1972	3.6491	-1.4982	-2.1639	0.0079	4.9017	-2.6335	2.1625	-2.0727	0.6306	
LA	0	10	8.23000	11.6727	-1.4495	-0.1148	-0.7551	0.8494	0.0014	*	5.1147	-2.5016	1.0445	-0.3135	0.0033	0.0033	
CE	0	1	8.18000	12.2040	-2.5463	0.1737	0.2227	0.0019	*	5.4306	-1.8832	0.2177	0.0036	0.0036			
TB	0	4	7.30000	12.3059	-2.0468	0.8646	-0.4632	0.0028	*	5.2774	-1.8882	0.2103	0.0035	0.0035			
LU	0	4	7.19000	11.3207	1.1864	0.4146	-1.3218	0.9452	0.0015	*	4.9920	-2.0768	0.6594	-0.3362	0.0047	0.0047	
HF	0	7	8.19000	11.9286	-1.5389	-0.1005	0.3408	0.0039	*	4.6051	-2.1287	0.9011	-0.5178	0.0060	0.0060		
TA	0	8	8.20000	11.5041	-1.1746	-0.2797	-0.4067	C.6561	0.0028	*	5.1001	-2.8433	1.1738	0.5173	-0.8561	0.0033	
W	0	1	6.80000	11.3448	-2.0836	0.1727	-1.4810	1.3151	0.0036	*	5.1329	-1.8799	0.2718	0.0035	0.0035		
IR	0	2	3.64000	11.4550	-1.3926	0.0274	0.7416	-0.6759	0.0003	*	5.2391	-2.0423	0.5144	-0.1725	0.0028	0.0028	
PT	0	2	3.82000	11.9957	-0.8149	-0.3026	-0.1607	0.0023	*	4.6742	-2.0805	0.5513	-0.2019	0.0028	0.0028		
PB	0	4	3.83000	10.7139	-1.1615	-0.3056	2.4034	-2.2780	0.0033	*	4.8570	-2.3241	1.3926	-1.6743	0.8970	0.0016	
BI	0	6	3.47000	10.7684	-0.2412	-0.6923	0.1559	0.0013	*	5.2349	-2.5169	1.2737	-0.6580	0.0027	0.0027		
TH	0	12	9.00000	11.8865	-1.6229	-0.1214	0.4378	0.0023	*	4.9201	-2.8341	1.2323	-0.1963	0.0049	0.0049		
B	0	+	1	11.5794	-0.7733	-0.0834	-0.3266	0.0026	*	3.6885	-1.7629	0.3487	0.0040	0.0040			
S ₁	0	+	1	4.9800	11.2473	-0.8817	0.0457	-0.3613	0.0010	*	4.5081	-1.8318	0.2842	0.0041	0.0041		
P	0	+	1	8.41000	11.2658	-0.9964	0.5314	-0.6840	0.0020	*	4.1845	-1.8326	0.3220	0.0038	0.0038		
S	0	+	1	5.43000	11.0273	-0.8558	0.0181	-0.3788	0.0007	*	4.7317	-1.8175	0.2998	0.0041	0.0041		

TABLE 5—Continued

MOL.	N STATES	DD (EV)	EQUILIBRIUM CONSTANT					PARTITION FUNCTION					MAX. ER.		
			B1	B2	B3	B4	B5	MAX.* ER.*	A0	A1	A2	A3			
AS	0 +	2	11.1821	-0.9353	0.5125	-0.6106	0.0015	*	4.4220	-1.9221	0.3190	0.0024	0.00019		
TA	0 +	2	11.4231	-2.0246	0.5461	-0.6106	0.0022	*	4.8366	-1.9527	0.3536	0.0019	0.00019		
LI	F	1	5.9100	10.6814	-0.5892	0.2241	-1.3376	0.8831	0.0020	*	4.1338	-2.1584	0.6294	-0.1988	
BE	F	4	5.8500	10.3864	-0.7484	0.1660	-0.5775	0.0043	*	4.2335	-1.9614	0.4093	0.0024	0.00024	
8	F	2	7.0800	11.5877	-0.5738	0.5283	0.0036	*	3.8857	-1.9781	0.5889	-0.1808	0.0037		
NA	F	1	5.3300	10.4112	-0.4247	0.4866	-2.4486	1.9135	0.0051	*	4.8566	-2.2801	0.5730	-0.1449	
MG	F	4	4.7500	10.0433	-0.5350	0.2486	-1.4962	1.0741	0.0027	*	4.9332	-2.1380	0.5065	-0.1498	
AL	F	7	6.8900	11.2299	-0.4816	-0.4865	0.0030	*	4.5405	-2.1033	0.6208	-0.2930	0.0016		
SI	F	4	5.5700	10.6012	-0.6898	-0.3675	0.0037	*	5.0871	-2.0375	0.4478	-0.1243	0.0044		
P	F	6	10.6706	-0.6432	-0.4816	-0.2458	0.0031	*	5.0146	-2.0268	0.6802	-0.2215	0.0026		
S	F	3	3.3000	10.6907	-0.5464	-0.2122	0.0027	*	5.3092	-2.1406	0.1786	0.0017	0.00019		
CL	F	2	2.6173	11.1734	-0.0830	-1.6190	0.7791	0.1202	0.0056	*	4.6390	-2.5206	1.5058	-0.8835	
K	F	1	5.0700	10.2876	-0.7142	1.4151	-3.3953	2.1866	0.0030	*	5.1495	-2.2814	0.4132	0.0039	
CA	F	8	5.4800	9.9724	-1.0667	1.5919	-2.3628	C.9265	0.0034	*	5.2010	-2.2653	0.8941	-0.5384	
SC	F	9	6.1700	10.5981	-1.0171	1.1437	-0.8442	-C.1190	0.0044	*	5.6041	-2.3100	0.6409	-0.5196	
MN	F	2	4.3500	10.3577	-0.9194	1.4158	-2.9550	1.7349	0.0018	*	5.6080	-2.0214	0.2692	0.0030	
FE	F	1	11.2390	-1.0958	0.8629	-1.7929	0.9010	0.0015	*	5.3670	-2.0615	0.1453	0.0024		
N1	F	1	11.6924	-0.9714	-0.0625	-0.3389	0.0036	*	4.9604	-1.8995	0.1930	0.0033	0.0001		
CU	F	4	4.4200	10.0113	-0.7175	0.0832	-0.2180	0.0037	*	4.8370	-2.2884	0.8728	-0.4688		
ZN	F	1	10.1169	-0.5424	-0.1226	-0.2252	0.0027	*	5.0022	-2.0212	0.2605	0.0008	0.0008		
GA	F	2	5.9800	11.0703	-0.6115	-0.4239	-0.1917	0.0025	*	4.8351	-2.1309	0.5213	-0.2157		
GE	F	3	5.0000	10.7425	-0.7351	-0.5092	0.0041	*	5.3375	-2.2045	0.3369	-0.1743			
AS	F	6	4.2000	10.5800	-0.6139	-0.1061	0.3669	-0.5674	0.0027	*	5.2767	-2.2834	0.7368	-0.3787	
SE	F	4	3.2100	10.7906	-0.9333	-0.1573	0.0022	*	5.2954	-1.8972	0.1966	0.0033	0.0003		
BR	F	3	2.5480	11.0229	-0.1576	-1.5765	1.1875	-0.1602	0.0054	*	4.8590	-2.5308	1.5162	-0.9432	
RB	F	1	5.0000	10.2442	-0.7236	1.3027	-2.9490	1.8249	0.0021	*	5.3264	-2.2828	0.3908	0.0032	
SR	F	5	5.5800	9.9281	-1.2447	2.2363	-3.2305	1.3573	0.0038	*	5.3982	-2.3020	0.8817	-0.5139	
Y	F	11	6.2000	10.6024	-1.0490	1.1985	-0.1664	-0.7350	0.0052	*	5.6990	-2.4244	0.4447	-0.5689	
AG	F	1	3.6400	10.4871	-0.3791	-0.4005	0.0023	*	5.0569	-1.6795	0.4621	-0.1498	0.0012		
CD	F	1	3.2000	9.9569	-0.6087	-0.2032	0.0034	*	5.2937	-1.9271	0.1470	0.0026	0.0004		
IN	F	3	5.2500	10.8279	-0.6921	-0.9794	0.6273	0.0016	*	5.0395	-2.1957	0.6631	-0.3618		
SN	F	3	4.9000	10.5104	-0.9423	-0.8303	0.4075	0.0015	*	5.4569	-2.3562	0.3650	-0.2188		
SB	F	4	4.4000	10.5298	-0.5245	0.1505	-0.0979	0.0040	*	5.4031	-2.4107	0.4508	-0.2383		
I	F	3	2.8790	10.3583	-0.1890	-2.3819	-7.7919	4.3837	-4.3614	0.0037	*	5.0315	-2.8144	-1.3055	-0.1345
CS	F	1	5.1500	10.2669	-1.2115	2.4490	-3.5500	1.4989	0.0060	*	5.4037	-2.2654	0.3684	0.0036	
BA	F	9	6.0500	10.1600	-2.0267	0.7124	3.0879	-3.4197	0.0055	*	5.5142	-2.4761	1.2354	-0.7552	
LA	F	1	11.7253	-2.0523	0.6883	-3.3671	0.0028	*	4.9748	-1.9224	0.1553	0.0028	0.0004		
HO	F	1	5.5700	11.3855	-2.3428	2.4802	1.8541	-8.1405	5.3461	0.0012	*	5.4368	-2.0523	0.2925	0.0022
YB	F	1	4.8000	9.9282	-1.1034	3.0140	-6.3465	4.0162	0.0049	*	5.4001	-2.1404	0.3367	0.0041	
LU	F	6	11.2570	-0.9711	-0.1425	-0.1458	-0.5448	0.5895	0.0017	*	4.9710	-2.2379	1.1473	-0.1335	
HG	F	1	1.8000	9.8844	-0.4512	-0.0824	-0.2834	0.0032	*	5.4072	-2.0889	0.0694	0.0028		
TL	F	3	4.5700	10.5151	-0.7422	-0.1678	0.7062	-0.7394	0.0009	*	5.1643	-2.1992	0.5398	-0.2303	
PB	F	3	3.6400	10.0314	-1.1454	0.2111	1.2319	-1.4696	0.0027	*	5.4584	-2.3244	0.7267	-0.2992	
LJ	NA	1	9.0737	-0.5315	2.3446	-5.3752	3.4409	0.0032	*	5.3162	-2.8055	2.1345	-0.2319		
AU	SI	3	3.2400	9.9729	-0.9545	0.5857	0.3695	-0.8312	0.0013	*	6.1485	-2.2354	0.1414	0.0043	
AS	P	2	10.8905	-1.1459	1.0654	-0.5237	-0.4253	0.0039	*	5.0912	-2.0238	0.2672	0.0025		
SB	P	1	3.6800	10.7736	-1.1956	1.0636	-0.3134	-0.5643	0.0034	*	5.3090	-2.0455	0.2420	0.0017	
BE	S	4	3.8000	10.4512	-0.0175	-0.6182	-1.5058	1.4841	0.0034	*	4.4452	-2.7285	1.4078	-0.4308	
B6	S	3	6.0100	11.2320	-0.5508	-0.8565	0.8903	-0.6407	0.0009	*	4.5362	-2.1517	0.9718	-0.5048	
MG	S	2	2.4000	10.2940	-0.6300	0.4199	-1.5174	1.0027	0.0025	*	5.0367	-2.1625	0.4859	-0.1780	

TABLE 5—Continued

MOL.	N	EQUILIBRIUM CONSTANT						PARTITION FUNCTION						MAX. ER.*	
		DD (EV)	B0	B1	B2	B3	B4	B5	A0	A1	A2	A3	A4		
AL S	4	3.8400	10.8924	-0.5704	-0.3551	-0.2837	-0.2058	-0.1437	-0.0943	-0.0531	-0.0311	-0.0190	-0.0079	0.0029	
SI S	1	6.4200	11.5515	-0.8733	0.0208	-0.2837	-0.2058	-0.1437	-0.0943	-0.0531	-0.0311	-0.0190	-0.0079	0.0017	
P S	5	4.5400	10.6659	-0.9384	0.5114	-0.4626	0.0040	*	0.0040	*	0.0022	*	0.0017	0.0036	
CA S	2	3.4600	10.3046	-1.2540	2.1302	-3.0765	1.2869	0.0553	0.0035	*	0.0035	*	0.0022	0.0014	
SC S	2	4.9200	11.2016	-1.3356	1.4964	-1.4560	0.4061	-0.2058	-0.1747	0.5336	-0.2470	0.4490	-0.1602	0.0018	
TI S	6	4.7500	11.1227	-1.4043	0.9862	-0.7360	0.0039	*	0.0039	*	0.0027	*	0.0019	0.0018	
CR S	2	3.3700	10.5115	-1.6188	1.8144	-1.4166	0.0032	*	0.0032	*	0.0018	*	0.0015	0.0015	
MN S	2	2.8500	10.4506	-1.0009	1.4933	-2.8376	1.5845	0.0015	*	0.0015	*	0.0020	*	0.0020	
CUS	3	2.8000	10.1393	-0.9778	0.9007	-0.7035	0.0023	*	0.0023	*	0.0018	*	0.0036	0.0036	
GE S	1	5.6700	11.3974	-1.0450	0.2535	-0.2691	0.0024	*	0.0024	*	0.0011	*	0.0011	0.0011	
AS S	2	3.7000	10.9106	-0.9360	0.3232	-0.1437	-0.6247	0.0026	*	0.0026	*	0.0030	*	0.0030	
SE S	4	4.3600	10.5005	-1.8227	0.2802	-0.2420	0.0042	*	0.0042	*	0.0037	*	0.0037	0.0037	
SR S	2	3.4800	10.2823	-1.5340	2.9746	-3.9940	1.6135	0.0049	*	0.0049	*	0.0033	*	0.0033	
Y S	1	5.4500	11.1927	-1.6274	1.7629	-0.2377	0.0054	*	0.0054	*	0.0025	*	0.0025	0.0025	
SN S	1	4.7700	11.1100	-1.3799	0.5722	0.3313	0.0053	*	0.0053	*	0.0017	*	0.0017	0.0017	
TE S	2	3.5000	10.6250	-0.8142	0.1980	0.4986	-0.6719	0.0005	*	0.0005	*	0.0025	*	0.0025	
HA S	4	4.3600	10.5005	-1.8227	0.1931	2.5675	-0.7377	-2.0641	0.0063	*	0.0063	*	0.0063	0.0063	
LA S	2	5.9100	11.4495	-1.9869	0.5209	-0.2144	0.0013	*	0.0013	*	0.0017	*	0.0017	0.0017	
PB S	4	3.4900	10.4773	-1.1713	-0.5003	2.7897	-2.4801	0.0034	*	0.0034	*	0.0027	*	0.0027	
BT S	2	3.1700	10.2889	-0.5804	-0.1945	0.0035	*	0.0035	*	0.0035	*	0.0016	*	0.0016	
L1 CL	1	4.8400	10.3223	-0.5527	0.2688	-1.5692	1.1464	0.0025	*	0.0025	*	0.0025	*	0.0025	
BE CL	3	10.0091	-0.6903	0.0756	-0.4330	0.0036	*	0.0036	*	0.0036	*	0.0029	*	0.0029	
B CL	3	5.5000	11.1693	-0.4633	-0.9362	1.0561	-0.7173	0.0009	*	0.0009	*	0.0061	*	0.0061	
NA CL	1	4.2300	10.1005	-0.4344	0.7696	-3.0544	2.3313	0.0047	*	0.0047	*	0.0044	*	0.0044	
HG CL	3	3.2900	9.7146	-0.5162	0.2041	-1.4277	1.1064	0.0028	*	0.0028	*	0.0018	*	0.0018	
AL CL	4	5.1200	10.8455	-0.3966	-0.7300	0.3184	0.0034	*	0.0034	*	0.0033	*	0.0027	*	0.0027
SI CL	4	10.5520	-0.6176	-0.3907	0.1392	0.0012	*	0.0012	*	0.0012	*	0.0014	*	0.0014	
P CL	2	10.3949	-0.8014	0.2807	-0.4320	0.0012	*	0.0012	*	0.0012	*	0.0024	*	0.0024	
K CL	1	4.3400	9.9707	-0.7106	1.6598	-3.9857	2.6197	0.0030	*	0.0030	*	0.0016	*	0.0016	
CA CL	8	4.0900	9.6477	-1.0163	1.5882	-2.6090	1.2516	0.0026	*	0.0026	*	0.0049	*	0.0049	
SC CL	5	3.4000	11.1185	-0.9624	0.6686	-0.7441	0.0030	*	0.0030	*	0.0030	*	0.0042	*	0.0042
MN CL	2	3.7000	10.1435	-1.0149	1.6196	-3.2245	1.9546	0.0020	*	0.0020	*	0.0020	*	0.0020	
FE CL	1	11.0006	-1.1059	0.7944	-1.5902	0.8381	0.0015	*	0.0015	*	0.0015	*	0.0027	*	0.0027
CU CL	8	3.9300	10.4843	-0.6643	-0.3641	0.9992	-0.9476	0.0023	*	0.0023	*	0.0017	*	0.0017	
ZN CL	1	2.1000	9.8821	-0.5316	-0.1244	-0.1776	0.0034	*	0.0034	*	0.0034	*	0.0015	*	0.0015
GA CL	3	4.9200	10.7355	-0.5423	-0.5943	0.4691	0.3717	0.0063	*	0.0063	*	0.0049	*	0.0049	
GE CL	4	4.4000	10.4551	-0.8067	-0.3883	0.3762	-0.4350	0.0014	*	0.0014	*	0.0014	*	0.0014	
AS CL	1	10.3224	-0.8430	0.3762	-0.4350	0.0014	*	0.0014	*	0.0014	*	0.0014	*	0.0014	
SE CL	1	10.7188	-0.9488	-0.1355	0.9992	-0.9476	0.0038	*	0.0038	*	0.0038	*	0.0038	*	0.0038
BR CL	2	2.2330	10.7561	-0.1150	-0.4691	0.6463	0.3717	0.0077	*	0.0077	*	0.0077	*	0.0077	
RB CL	1	4.3400	9.9564	-0.7119	1.6024	-3.5467	2.1773	0.0027	*	0.0027	*	0.0027	*	0.0027	
SR CL	4	4.1600	9.8012	-1.2949	2.3444	-3.4177	1.5467	0.0038	*	0.0038	*	0.0031	*	0.0031	
Y CL	2	11.0660	-1.2883	1.0142	-0.6058	-0.4580	0.0049	*	0.0049	*	0.0049	*	0.0028	*	0.0028
AG CL	2	3.2200	10.2885	-0.3907	-0.3742	0.0038	*	0.0038	*	0.0038	*	0.0038	*	0.0038	
CD CL	1	2.1200	9.8054	-0.5097	-0.2603	0.0009	*	0.0009	*	0.0009	*	0.0013	*	0.0013	
IN CL	3	4.4400	10.5285	-0.6450	-1.0931	0.7648	0.0013	*	0.0013	*	0.0012	*	0.0042	*	0.0042
SN CL	3	10.2282	-0.9403	-0.8195	0.4364	0.0013	*	0.0013	*	0.0013	*	0.0030	*	0.0030	
SB CL	2	10.3567	-0.8405	0.6204	-0.2841	0.0035	*	0.0035	*	0.0035	*	0.0012	*	0.0012	
TE CL	1	10.2457	-0.9424	0.0756	0.6943	-2.0504	7.5104	-5.2217	0.0018	*	0.0018	*	0.0021	*	0.0021
I CL	3	2.1531	10.5319	0.3459	-1.6943	-2.0504	0.0018	*	0.0018	*	0.0018	*	0.0084	*	0.0084

TABLE 5—Continued

MOL.	N STATES	EQUILIBRIUM CONSTANT						PARTITION FUNCTION						MAX. ER.*	
		D0 (EV)	B0	B1	B2	B3	B4	B5	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	
BA CL	10	4.5500	9.9594	-1.9957	0.9232	-2.2392	-2.6168	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	0.0008	0.0008	
AU CL	1	3.5000	10.4912	-0.9692	0.4074	-0.2975	0.0038	*	5.5640	-2.0253	0.2002	0.0002	0.0002	0.0002	
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	0.0013	
TL CL	2	3.8200	10.2434	-0.7136	-0.0901	0.0751	0.0039	*	5.7692	-2.2258	0.4817	-0.2245	0.0010	0.0010	
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	0.0024	0.0024
AL SE	2	3.4600	10.7857	-0.7858	-0.1407	0.0027	*	5.4873	-2.0722	0.2604	0.0006	0.0006	0.0006	0.0005	
SI SE	1	5.6400	11.3895	-0.9755	-0.0901	0.0023	*	5.1075	-2.0100	0.2322	0.0001	0.0001	0.0001	0.0001	
CU SE	3	2.5500	10.0783	-0.9688	-0.6674	0.0018	*	6.1556	-2.3030	0.1452	0.0023	0.0023	0.0023	0.0023	
GE SE	1	4.9800	11.2384	-1.1163	-0.3775	0.0015	*	5.5644	-2.0873	0.2463	0.0005	0.0005	0.0005	0.0005	
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	0.0013	
SI TE	1	4.6400	11.1445	-1.0274	0.2402	-0.1432	0.0036	*	5.3406	-1.9922	0.1831	0.0027	0.0027	0.0027	
GE TE	1	4.2400	11.0317	-1.1431	-0.0535	0.0317	0.0039	*	5.8258	-2.0901	0.2184	0.0007	0.0007	0.0007	
K I	1	3.3100	9.6625	-0.7210	1.8703	-3.9239	2.5006	0.0028	*	6.1888	-2.3327	0.2099	0.1594	0.0052	
H H	1	4.4781	11.1759	-0.8735	-0.7470	0.2748	0.0007	*	1.6498	-1.6265	0.7472	-0.251	0.0007	0.0007	
H H +	1	2.6508	9.9835	-0.0664	-1.4979	-0.0195	C.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	-2.0989	0.6310	0.0029	0.0029	0.0029	0.0029	
LJ LI	4	1.0460	9.4736	-0.3244	1.1962	-3.5541	2.4491	0.0030	*	4.6515	-2.5580	0.5835	0.0041	0.0041	0.0041
B B	2	3.0200	11.0585	-0.4932	-0.3893	0.0029	*	4.2793	-2.0492	0.4345	0.0029	0.0029	0.0029	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	0.0012	0.0012	
C C +	1	5.3200	11.4535	-0.7842	-0.0300	-0.3124	0.0004	*	4.1166	-1.8188	0.2984	0.0041	0.0041	0.0041	
N N	1	9.7594	11.8838	-0.8915	0.2929	-1.4220	0.9007	0.0009	*	3.2643	-1.7303	0.4192	0.0025	0.0025	0.0025
N N +	4	8.7128	11.8052	-0.4492	-0.5843	-0.9278	0.8821	0.0018	*	3.6830	-2.1583	0.9929	-0.2181	0.0031	0.0031
O O	6	5.1156	11.8058	-0.5309	-0.6244	0.0011	*	4.0363	-2.0779	0.7660	-0.2111	0.0016	0.0016	0.0016	
O O +	2	6.6630	11.5549	-0.7335	-0.3005	-0.1753	0.0007	*	4.0194	-1.8480	0.4661	0.0027	0.0027	0.0027	
F F	1	1.6020	11.6249	-0.3917	-0.5115	-0.1205	0.0030	*	4.0355	-2.1726	0.4608	0.0036	0.0036	0.0036	
NE NE +	1	1.3000	10.2518	-0.6359	-0.2103	0.0027	*	4.6665	-1.9305	0.1411	0.0017	0.0017	0.0017		
NA NA	4	0.7200	9.2096	-0.1176	1.1635	-5.6561	8.6389	-4.7450	0.0028	*	5.6752	-2.6810	0.6626	-0.1283	
MG MG	2	0.0501	8.6463	-1.6726	1.6431	-3.3322	2.4266	0.0044	*	5.6533	-1.0891	0.1211	-0.1854	0.0008	
AL AL	2	1.5500	10.3474	-0.2333	-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	-0.3694	0.8076	-0.8107	0.0009	*	5.2617	-2.1485	0.5647	-0.2985	0.0037	
P P	4	5.0330	11.2490	-0.9821	0.2336	0.8887	-1.3142	0.0050	*	4.9884	-2.1415	1.1375	-1.8111	1.2263	
P P +	6	4.9900	10.7616	-0.8035	0.3322	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	0.0030	0.0030	
S S +	1	5.3700	10.9811	-0.9318	0.4797	-0.6452	0.0019	*	5.0598	-1.8928	0.2034	0.0034	0.0034	0.0034	
CL CL	1	2.4794	11.2793	-0.5356	-0.4665	0.0032	*	4.7438	-2.1109	0.3280	0.0033	0.0033	0.0033		
K K	4	0.5140	8.9949	-1.1018	3.7043	-6.1302	3.2656	0.0037	*	6.2963	-2.3873	0.2118	0.0041	0.0041	0.0041
CU CU	3	2.0300	10.1749	-0.9712	1.1405	-0.8963	0.0040	*	5.4806	-2.4706	0.8867	-0.4736	0.0018	0.0018	
AS AS	5	3.9600	11.0864	-0.7253	-0.2214	1.2187	-1.1896	0.0025	*	5.2506	-2.4520	1.5981	-1.9349	0.9330	
SE SE	2	3.0900	11.0950	-0.9844	0.0343	0.2123	0.0006	*	5.7320	-2.1070	0.0023	0.0023	0.0023	0.0023	
SB SB	1	3.0900	11.0023	-1.2817	1.1014	0.0151	-0.7954	0.0032	*	5.7012	-2.0571	0.1630	0.0012	0.0012	0.0012
TE TE	2	2.6770	10.7951	-0.7579	0.4198	0.9161	-1.1418	0.0006	*	6.1915	-2.4514	0.0164	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	0.0028	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
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	MAX.E.	PARTITION FUNCTION				ELEMENT	MAX.E.	PARTITION FUNCTION			
		C0	C1	C2	C3			C0	C1	C2	C3
H	0.00000	0.30103	-0.00001	BR+	0.00254	0.82697	-0.30362	0.17411	-2.50288	1.24577	
H +	0.00000	0.00000	0.00000	PB	0.00238	1.35139	-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	1.07605	-0.90007	1.71783	-1.32443		
LI	0.00128	0.31804	-0.20816	ZR	0.00078	1.51403	-1.10749	0.71584	-0.30517		
BE	0.00619	0.00801	-0.17135	NB	0.00093	1.72793	-0.96931	0.84701	-0.77242		
BE +	0.00289	0.30389	-0.08819	RU	0.00259	1.53544	-0.95790	0.65520	-0.19002		
B	0.00319	0.78028	-0.01622	RH	0.00403	1.42145	-0.73846	0.28160			
B +	0.00377	0.00349	-0.01035	PD	0.00548	0.46919	-1.51528	0.26006	2.97576	-2.29501	
C	0.00375	0.96752	-0.09452	AG	0.00379	0.30488	-0.01088				
C +	0.00284	0.77239	-0.02540	CD	0.00000	0.00000	0.00000				
N	0.00279	0.60683	-0.08674	IN	0.00262	0.61694	-0.3160	-0.28054	0.29267		
N +	0.00362	0.94968	-0.06463	SN	0.00342	0.71534	-0.76319	-0.44970	0.4099		
O	0.00325	0.95033	-0.05703	SB	0.00314	0.67754	-0.39920	0.64590	-0.31914		
O +	0.00307	0.60405	-0.03025	TE	0.00203	0.79722	-0.32317	0.26550			
F	0.00072	0.76284	-0.0582	I	0.00191	0.62732	-0.10487	0.10197			
NE	0.00000	0.00000	0.00000	CS	0.00710	0.40691	-0.96438	2.87484	-3.24127	1.10631	
NE +	0.00033	0.74847	-0.06562	BA	0.00534	0.40430	1.93697	2.13100	1.56692	-2.64798	
NA	0.00328	0.30955	-0.17778	LA	0.00302	1.43627	-1.44018	0.81057	-0.23872		
MG	0.00239	0.00556	-0.12840	CE	0.00170	2.28510	-1.87742	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	-0.0207	HO	0.00813	1.54615	-1.77233	2.45212	0.48439	-1.98287	
AL +	0.00365	0.00334	-0.00995	YB	0.00512	0.49819	-0.69224	3.49819	-6.64720	4.20480	
SI	0.00318	0.97896	-0.9208	LU	0.00231	0.94528	-0.67678	1.02821	-2.06203	1.54988	
SI +	0.00199	0.75647	-0.05490	HF	0.00337	1.16596	-1.11790	0.69486			
P	0.00179	0.64618	-0.31132	TA	0.00266	1.23539	-1.44778	0.84884			
P +	0.00094	0.93588	-0.8848	TA +	0.00081	1.36131	0.29035	0.13472	0.34727		
S	0.00376	0.95254	-0.15166	W	0.00348	1.11208	-1.41233	0.27987	-1.21831	1.28689	
S +	0.00251	0.61974	-0.1465	IR	0.00349	1.31959	-0.83851	0.55564			
CL	0.00041	0.74465	-0.07389	PT	0.00057	1.29756	-0.34013	0.17630	-0.25884		
CL +	0.00339	0.92728	-0.15913	AU	0.00381	0.38900	-0.4824	0.68902	-0.31529		
K	0.00209	0.34419	-0.48157	HG	0.00132	0.00120	-0.00360				
CA	0.00388	0.07460	-0.75759	HG +	0.00168	0.30262	0.00465				
SC	0.00581	1.08209	-0.77814	TL	0.00325	0.38523	-0.36653				
TI	0.00244	1.47343	-0.97220	PB	0.00302	0.19574	-0.92697	0.99476	0.82393	-1.33084	
V	0.00434	1.68359	-0.82055	RI	0.00173	0.62814	-0.20692	0.50277	-0.37664		
CR	0.00449	1.02332	-1.02540	TH	0.00633	1.42677	-1.89720	1.03185	0.33964		
MN	0.00201	0.80810	-0.39108	U	0.00299	1.93666	-2.05483	0.90354	2.82611	-2.77207	
FE	0.00382	1.44701	-0.61040								
CO	0.00436	1.52929	-0.71430								
NI	0.00392	1.49063	-0.33662								
CU	0.00209	0.36884	-0.46740								
ZN	0.00284	-0.00147	-0.02804								
ZN +	0.00024	0.30123	-0.00062								
GA	0.00466	0.71314	-0.21023								
GE	0.00420	0.88280	-0.0360								
AS	0.00197	0.65368	-0.33297								
AS +	0.00282	0.77362	-0.56486								
SE	0.00198	0.87375	-0.29536								
BR	0.00322	0.66881	-0.15099								

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 ${}^P K$ 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:

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

We express our sincere thanks to L. Devos for having punched all molecular data of the present investigation from Huber and Herzberg's tables. We also thank very much H. Van Diest for his help in all numerical calculations and particularly for the fitting by the minimax method.

REFERENCES

- Aller, M. F., and Everett, C. H. M. 1972, *Ap. J.*, **172**, 447.
- Barrodale, I., and Young, A. 1966, *Numer. Math.*, **8**, 295.
- Bohn, H. U., and Wolf, B. E. 1984, *Astr. Ap.*, **130**, 202.
- Bolton, C. T. 1970, *Ap. J.*, **161**, 1187.
- Chase, R. C., et al. 1974, *J. Phys. Chem. Ref. Data*, **3**, 311.
- _____. 1975, *J. Phys. Chem. Ref. Data*, **4**, 1.
- _____. 1978, *J. Phys. Chem. Ref. Data*, **7**, 793.
- Colket, M. B. 1984, *J. Quant. Spectrosc. Rad. Transf.*, **31**, 7.
- de Galan, L., Smith, R., and Winefordner, J. B. 1968, *Spectrochimica Acta*, **22B**, 521.
- Gibson, G. E., and Heitler, W. 1928, *Zs. Phys.*, **49**, 465.
- Gurvich, L. V., et al. 1962, in *Thermodynamic Properties of Individual Substances*, Vol. 2, *Tables of Thermodynamic Constants*, ed. V. P. Glushko et al. (Moscow: Soviet Acad. Sci.), p. 830.

- Gurvich, L. V., et al. 1978–1981, *Termo-dinamicheskie Svoistva Individuálnikh Veschev*, Vols. 1–3 ed. V. P. Glushko et al. (Moscow: Soviet Acad. Sci.).
- Huber, K. P., and Herzberg, G. 1979, *Constants of Diatomic Molecules* (New York: Van Nostrand).
- Irwin, A. W. 1981, *Ap. J. Suppl.*, **45**, 621.
- Kurucz, R. L. 1970, *Atlas — A Computer Program for Computing Model Stellar Atmospheres* (Smithsonian Ap. Obs. Spec. Rep., No. 309).
- Murad, E., and Hildenbrand, D. L. 1975, *J. Chem. Phys.*, **63**, 1133.
- Phillips, J. G., and Davis, S. P. 1979, *Ap. J.*, **229**, 867.
- Russell, H. N. 1934, *Ap. J.*, **79**, 317.
- Sarychev, A. P. 1980, *Astr. Zh.*, **57**, 1020 (English transl. *Soviet Astr.*, **24**, 586 [1980]).
- Sauval, A. J. 1972, Ph.D. thesis, Université de Liège.
- Scalo, J. M., and Ross, J. E. 1976, *Astr. Ap.*, **48**, 219.
- Schadee, A. 1968, *Ap. J.*, **151**, 239.
- Schlender, B., and Traving, G. 1965, *Zs. Ap.*, **61**, 92.
- Shankar, A., and Littleton, J. E. 1983, *Ap. J.*, **274**, 916.
- Stull, D. R., and Prophet, H. 1971, *JANAF Thermochemical Tables*, NSRDS, NBS Pub. No. 37 (2d ed.; Washington: National Bureau of Standards).
- Tarafdar, S. P. 1977, *J. Quant. Spectrosc. Rad. Transf.*, **17**, 537.
- Tatum, J. B. 1966, *Pub. Dom. Ap. Obs. Victoria*, **13**, 1.
- Traving, G., Baschek, G., and Holweger, H. 1966, *Abh. Hamburger Sternw.*, **8**, 1.
- Tsuji, T. 1964, *Ann. Tokyo Astr. Obs.*, **9**, 1.
- _____. 1973, *Astr. Ap.*, **23**, 411.
- Van Diest, H. 1980, *Astr. Ap.*, **83**, 378.
- Vardya, M. S. 1966, *M.N.R.A.S.*, **134**, 347.
- Witschel, W. 1974, *J. Chem. Soc. Faraday Trans. II*, **70**, 1441.

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