

# Appendix A

## Spectral Terms for Atoms and Molecules

In previous chapters, the calculation of the electronic partition function of atomic hydrogen has been carried out by using the analytical formulation of the energy levels and of the corresponding statistical weights. The situation is deeply different when dealing with the multielectron atoms. In principle, one can write the Schrödinger equation for the system and solve it through numerical methods. This approach is in general followed for the ground state and for the so-called *low-lying* excited states, i.e., for electronic states arising from the rearrangement of valence electrons. On the other hand, the solution of the Schrödinger equation for *high-lying* excited states (i.e., states characterized by values of principal quantum number different from that of the ground state) is still a prohibitive task despite the enormous progress of quantum chemistry calculations. In this case, semiempirical methods, based on known electronic levels, can be used to get a complete set of energy levels, ready for the cutoff criterion. In doing so, we must be aware of the enormous number of energy levels arising from the coupling of the angular and spin momenta in the multielectron systems. This kind of problems will be analyzed in the first part of this appendix that will give us the recipes to get complete sets of energy levels for multielectron atoms.

In the second part, we will consider similar problems for diatomic molecules.

### A.1 Atomic Electronic Terms

The electrons in multielectron atoms can be identified through four quantum numbers (principal, angular, magnetic, and spin) in the order

$$\begin{aligned}(n_1, l_1, m_1, s_1) \\ (n_2, l_2, m_2, s_2) \\ (n_3, l_3, m_3, s_3) \\ \dots\end{aligned}$$

In the frame of the *vector model* for angular momentum, let us define the following total quantities:

- $L$  Quantum number for the *orbital* angular momentum, associated to the squared modulus of the vector  $\mathbf{L}$ , i.e.  $|\mathbf{L}|^2 = L(L + 1)$ , with  $(2L + 1)$  values of the projection on the quantization axis (the  $z$ -axis)  $M_L = -L, -L + 1, \dots, 0, \dots, L - 1, L$ .
- $S$  Quantum number associated to the *spin* angular momentum, corresponding to a vector  $\mathbf{S}$  with modulus  $|\mathbf{S}|^2 = S(S + 1)$ , with  $(2S + 1)$  values of the projection on the quantization axis  $M_S = -S, -S + 1, \dots, 0, \dots, S - 1, S$ .
- $J$  Total angular momentum for  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  with  $|\mathbf{J}|^2 = J(J + 1)$ .

The sum rules are those of vector addition, considering their possible relative orientation. In the following, we will present the practical rules for obtaining  $L$ ,  $S$  and  $J$ <sup>1</sup>.

### A.1.1 Calculation of $L$

One-electron atoms  $L_1 = \ell_1$ .

Two-electron atoms  $L_2$  assumes all the integer values in the interval  $\ell_1 + \ell_2, \ell_1 + \ell_2 - 1 \dots |\ell_1 - \ell_2|$

Three-electron atoms  $L_3$  assumes, for each possible value of  $L_2$ , all the values in the interval  $L_2 + \ell_3, L_2 + \ell_3 - 1 \dots |L_2 - \ell_3|$ .

The procedure is extended adding one electron at a time.

### A.1.2 Calculation of $S$

One-electron atoms  $S_1 = s_1$

Two-electron atoms  $S_2$  assumes all the integer values in the interval  $s_1 + s_2, s_1 + s_2 - 1 \dots |s_1 - s_2|$

Three-electron atoms  $S_3$  assumes, for each possible value of  $S_2$ , all the values in the interval  $S_2 + s_3, S_2 + s_3 - 1 \dots |S_2 - s_3|$ .

The procedure is extended adding one electron at a time.

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<sup>1</sup>It should be noted that the scheme presented in this chapter is the so-called Russell–Saunders coupling scheme, widely used for the derivation of atomic term symbols of light atoms ( $Z \lesssim 40$ ). Alternatively, the  $j - j$  coupling scheme can be considered. Within this frame, the orbital and spin angular momenta of each electron are coupled ( $j_i = \ell_i + s_i$ ) and then the coupling of one-electron total angular momenta ( $j_1, j_2, j_3 \dots$ ) results in the total angular momentum of the atom  $J$ . This scheme is more appropriate for heavy atoms, when the spin-orbit coupling is the relevant interaction.

### A.1.3 Calculation of $J$

$J$  can assume, for each possible value of  $L$  and  $S$ , all the integer values in the range  $L + S, L + S - 1 \dots |L - S|$ .

Before passing to practical examples, we want to remind that each electronic term, corresponding to a given electronic configuration, is characterized by a *term symbol* written in the form  $^{2S+1}L_J$ . Capital letters in the series ( $S, P, D, F, G, \dots$ ) correspond to different values of the orbital angular momentum  $L$  (0, 1, 2, 3, 4,  $\dots$ ). On the left of the capital letter, the value of spin multiplicity  $2S + 1$  is reported<sup>2</sup>, while on the right the value of  $J$  is found. The total multiplicity of the state, i.e., the statistical weight is  $2J + 1 = (2L + 1)(2S + 1)$ . Therefore,

$^2S_{1/2}$  identifies a state with  $L = 0$  (state  $S$ ), total spin  $S = \frac{1}{2}$ , resulting in a *doublet* (multiplicity  $2S + 1 = 2$ ) and with  $J = \frac{1}{2}$  ( $J = L + S = 0 + \frac{1}{2} = \frac{1}{2}$ ). The statistical weight of the state is  $2J + 1 = 2$ .

#### A.1.3.1 Hydrogen

For  $n = 1$  (ground state,) we have  $H(1s)$  which corresponds to

$$\begin{aligned} S &= s_1 = \frac{1}{2} \\ L &= \ell_1 = 0 \\ J &= \frac{1}{2}. \end{aligned}$$

The electronic term is written as  $^2S_{1/2}$ . The statistical weight is given by  $g_1 = 2J + 1 = 2$  having energy  $\varepsilon_1 = 0$ .

For  $n = 2$ , we have  $H(2s)$  and  $H(2p)$  states. The angular momentum of  $H(2s)$  is analogous to the  $H(1s)$  and therefore the electronic term is  $^2S_{1/2}$  and the statistical weight is  $g_{2s} = 2$ .

Let us now consider the excited state  $H(2p)$

$$\begin{aligned} S &= s_1 = \frac{1}{2} \\ L &= \ell_1 = 1 \\ J &= \left\{ \frac{3}{2}, \frac{1}{2} \right\}. \end{aligned}$$

Therefore, we have two terms  $\{^2P_{3/2}, ^2P_{1/2}\}$  with statistical weights of 4 and 2, respectively. The energy of the state is given by

$$\varepsilon_2 = I_H \left( 1 - \frac{1}{2^2} \right) = \frac{3}{4} I_H$$

independently of the angular momentum<sup>3</sup>. Therefore, summing the contribution of the three terms we have  $g_{n=2} = 2 + 4 + 2 = 8$ , in agreement with the general formula  $g_n = 2n^2$ .

<sup>2</sup>Depending on the spin multiplicity, electronic states of atoms are classified as *doublets* ( $2S + 1 = 2$ ), *triplets* ( $2S + 1 = 3$ ), *quartets* ( $2S + 1 = 4$ ),  $\dots$

<sup>3</sup>If the spin-orbit coupling is neglected.

### A.1.3.2 Helium

The ground state configuration is  $He(1s^2)$ . The two electrons are not independent because, due to the *Pauli exclusion principle*, their spins must be antiparallel. Therefore, we have:

$$\begin{aligned} L &= 0 \text{ being } \ell_1 = \ell_2 = 0 \\ S &= 0 \text{ being } s_1 = s_2 = \frac{1}{2} \text{ with } m_{s_1} = -m_{s_2} \\ J &= 0 \end{aligned}$$

giving a configuration  $^1S_0$ , corresponding to a *closed shell atom*, characteristic of noble gas ground state, having degeneracy  $g_1 = 1$ .

Let us consider the  $He(1s2s)$  excited configuration. The two electrons are now independent because they do not occupy the same orbital. Therefore, we have:

$$\begin{aligned} L &= 0 \text{ being } \ell_1 = \ell_2 = 0 \\ S &= \{1, 0\} \text{ being } s_1 = s_2 = \frac{1}{2} \\ J &= \{1, 0\} \end{aligned}$$

giving the configurations  $^3S_1$  and  $^1S_0$ , corresponding to a triplet ( $g = 3$ ) and a singlet ( $g = 1$ ) states.

### A.1.3.3 Two Not-Equivalent $p$ Electrons ( $np, mp$ )

The two electrons are independent because are not in the same orbital. Therefore:

$$\begin{aligned} L &= \{2, 1, 0\} \text{ being } \ell_1 = \ell_2 = 1 \\ S &= \{1, 0\} \text{ being } s_1 = s_2 = \frac{1}{2}. \end{aligned}$$

To calculate  $J$ , we have to combine the different contributions giving the following terms

$L$	$S$	$J$	Terms
2	1	{3,2,1}	$^3D_3, ^3D_2, ^3D_1$
2	0	2	$^1D_2$
1	1	{2,1,0}	$^3P_2, ^3P_1, ^3P_0$
1	0	1	$^1P_1$
0	1	1	$^3S_1$
0	0	0	$^1S_0$

### A.1.3.4 Two Equivalent $p$ Electrons ( $np^2$ )

For two equivalent  $p$  electrons, characterized by the same principal and orbital quantum numbers ( $n, \ell$ ), not all the electronic terms derived in the previous example do exist. In this case in fact the *Pauli exclusion principle* restricts the number of allowed configurations. For the configuration  $np^2$ , i.e. ( $\ell_i = 1, s_i = \frac{1}{2}$ , with

$m$												
1	↑↓	□	□	↑	□	↑	↑	□	↑	↑	□	↓
0	□	↑↓	□	↓	↑	□	↑	↑	□	↓	↓	□
-1	□	□	↑↓	□	↓	↓	□	↑	↑	□	↑	↑
$M_L$	2	0	-2	1	-1	0	1	0	-1	1	0	-1
$M_S$	0	0	0	0	0	0	1	1	1	0	0	0
	${}^1D_2$					${}^1S_0$	${}^3P_{2,1,0}$					

Fig. A.1 Arrangements of two electrons on three equivalent  $p$  orbitals

axial projections  $m_{\ell_i} = \pm 1, 0$ ,  $m_{s_i} = \pm \frac{1}{2}$ ), let us consider the possible values of the electrons angular momentum projections, algebraically summing in the resulting total angular and spin momentum projections,  $M_L = m_{\ell_1} + m_{\ell_2}$  and  $M_S = m_{s_1} + m_{s_2}$ , as shown in Fig. A.1, where uparrows correspond to  $m_s = \frac{1}{2}$  and downarrows to  $-\frac{1}{2}$ . The configurations originating negative total spin projection are implicitly included.

The maximum  $M_L$  value of 2, found in constructing the allowed configurations, with maximum  $M_S = 0$ , implies the existence of a term  ${}^1D$ , thus accounting for five configurations with  $(M_L = \pm 2, \pm 1, 0$  and  $M_S = 0)$ . Repeating the procedure on the remaining configurations,  $(M_L)_{\max} = 1$  and  $(M_S)_{\max} = 1$ , one accounts for a  ${}^3P$  term with nine configurations arising from allowed values  $M_L = \pm 1, 0$  and  $M_S = \pm 1, 0$ . Finally, the last arrangement ( $M_L = 0$  and  $S = 0$ ) leads to the  ${}^1S$  term. The *group theory* offers an elegant and compact derivation of allowed terms (Bishop 1993), though beyond the scope of this book. It can be demonstrated that the spatial wavefunction for  $D$  and  $S$  terms is even, while spin wavefunction is even for triplets and odd for singles. It is straightforward that due to the antisymmetric nature of the total (spatial+spin) electronic wavefunction, only  ${}^1S, {}^1D$  and  ${}^3P$  terms could exist.

This is the case of ground and low-lying excited states of carbon atom.

Term	Energy (cm <sup>-1</sup> )	$g$
${}^3P_0$	0	1
${}^3P_1$	16.40	3
${}^3P_2$	43.40	5
${}^1D_2$	10,192.63	5
${}^1S_0$	21,648.01	1

### A.1.3.5 Three Not-Equivalent $p$ Electrons ( $n_1p, n_2p, n_3p$ )

The results of the two-electron case with configuration  $(L_2, S_2)$  must be combined with the third electron  $(l_3, s_3)$ , i.e.,

$L_2$	$\ell_3$	$L$	$S_2$	$s_3$	$S$
2	1	{3,2,1}	1	1/2	{3/2,1/2}
1	1	{2,1,0}	0	1/2	1/2
0	1	1			

Let us now compose  $L$  and  $S$ :

$L$	$S$	$J$	Terms	# of terms
3	3/2	{9/2,7/2,5/2,3/2}	${}^4F_{9/2,7/2,5/2,3/2}$	1
2	3/2	{7/2,5/2,3/2,1/2}	${}^4D_{7/2,5/2,3/2,1/2}$	2
1	3/2	{5/2,3/2,1/2}	${}^4P_{5/2,3/2,1/2}$	3
0	3/2	3/2	${}^4S_{3/2}$	1
3	1/2	{7/2,5/2}	${}^2F_{7/2,5/2}$	2
2	1/2	{5/2,3/2}	${}^2D_{5/2,3/2}$	4
1	1/2	{3/2,1/2}	${}^2P_{3/2,1/2}$	6
0	1/2	1/2	${}^2S_{1/2}$	2

### A.1.3.6 Three Equivalent $p$ Electrons ( $np^3$ )

It turns out (see Fig. A.2) that for  $np^3$  electronic configuration only the terms  ${}^4S$ ,  ${}^2D$ ,  ${}^2P$  survive. This is the case of the nitrogen atoms in ground and low-lying states with three electrons having principal quantum number  $n = 2$

Term	Energy (cm <sup>-1</sup> )	$g$
${}^4S_{3/2}$	0	4
${}^2D_{5/2}$	19224.464	6
${}^2D_{3/2}$	19233.177	4
${}^2P_{1/2}$	28838.920	2
${}^2P_{3/2}$	28839.306	4

$m$										
1	↑↓		↑		↑	↑↓	↑	↑	↑	↑
0	↑	↑	↑↓	↑↓	↑			↓	↑	↓
-1		↑↓		↓	↓	↑	↑↓	↑	↑	↓
$M_L$	2	-2	1	-1	0	1	-1	0	0	0
$M_S$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{1}{2}$
	${}^2D_{\frac{5}{2}, \frac{3}{2}}$					${}^2P_{\frac{3}{2}, \frac{1}{2}}$			${}^4S_{\frac{3}{2}}$	

Fig. A.2 Arrangements of three electrons on three equivalent  $p$  orbitals

**Table A.1** Electronic terms for atoms with equivalent-electron configurations

Configuration	Electronic terms	Atoms
$p p^5$	$^2P$	B, F
$p^2 p^4$	$^1S \ ^3P \ ^1D$	C, O, N <sup>+</sup>
$p^3$	$^4S \ ^2P \ ^2D$	N, O <sup>+</sup>
$p^6$	$^1S$	Ne
$d d^9$	$^2D$	Sc
$d^2 d^8$	$^1S \ ^3P \ ^1D \ ^3F \ ^1G$	Ti, Ni
$d^3 d^7$	$^2P \ ^4P \ ^2D \ ^2F \ ^4F \ ^2G \ ^2H$	V, Co
$d^4 d^6$	$^2^1S \ 2^3P \ 2^1D \ 3^3D \ 5^1D \ ^1F$ $^2^3F \ 2^1G \ 3^3G \ ^3H \ ^1I$	Fe
$d^5$	$^2S \ ^6S \ ^2P \ ^4P \ 3^2D \ ^4D \ 2^2F$ $^4F \ 2^2G \ ^4G \ ^2H \ ^2I$	Mn
$d^{10}$	$^1S$	Zn

### A.1.3.7 Four Equivalent $p$ Electrons ( $np^4$ )

This situation gives the same terms as the two equivalent  $p$  electrons. This is the case of the oxygen atoms in ground and low-lying excited states, having four electrons with principal quantum number  $n = 2$ , reported below

Term	Energy (cm <sup>-1</sup> )	$g$
$^3P_2$	0	5
$^3P_1$	158.265	3
$^3P_0$	226.977	1
$^1D_2$	15867.862	5
$^1S_0$	33792.583	1

In Table A.1, the electronic terms for equivalent-electron configurations are given. It should be noted that configurations having equal number of electrons or *electron-holes* have to be considered as equivalent, giving rise to the same electronic terms. Complete shell configurations, i.e.  $p^6$ , always give the  $^1S$  term. We give here the definition of the parity of atomic terms  $P = (-1)^{\sum_i \ell_i}$ , being the exponent the algebraic sum of orbital angular momenta of electrons, in a given electronic configuration.

## A.2 Complete Sets of Electronic Levels

The calculation of electronic partition function of atomic species needs of complete sets of energy levels and of corresponding statistical weights. Here, we want to present a very simple and rapid method based on the calculation of energy levels by an hydrogenic approximation and by calculating the statistical weight through the

L–S coupling. Some examples will explain the procedure which closely follows that one described in the previous pages. A better set of energy levels can be obtained by using semiempirical methods with the aid of existing tabulated energy levels (Capitelli and Molinari 1970) (see also Sect. A.3).

### A.2.1 Helium

We want to calculate the complete set of levels with energies and statistical weights for the configurations derived from the interaction of the Helium core ( ${}^2S$ ) with the (optical) electron jumping on the excited levels.

Let us start with the interaction

$${}^2S + 2s$$

We note that the core configuration ( $1s^1$ ) is characterized by quantum numbers  $S_{\text{core}} = 1/2$  and  $L_{\text{core}} = 0$ , while the  $2s$  excited electron has spin  $1/2$  and  $\ell = 0$ . In the frame of L-S coupling scheme, the singlet  ${}^1S_0$  ( $g = 1$ ) and triplet  ${}^3S_1$  ( $g = 3$ ) states are obtained.

Consider now the interaction

$${}^2S + 2p$$

i.e., ( $L_{\text{core}} = 0, S_{\text{core}} = 1/2$ ) + ( $\ell = 1, s = 1/2$ ). We obtain a triplet state ( $L = 1$ ), which corresponds to  ${}^1P_1$  ( $g = 3$ ),  ${}^3P_{2,1,0}$  ( $g = 9$ ) and the total statistical weight is  $g_{n=2} = 16$ .

Let us now consider the interaction of the core with one electron in the  $n = 3$  shell. The interactions with the  $3s$  and  $3p$  states follow directly from the cases above considered for the shell  $n = 2$ . Additionally, the interaction with the  $3d$  electron must be considered

$${}^2S + 3d$$

originating, in the L–S coupling,  ${}^1D_2$  ( $g = 5$ ) and  ${}^3D_{3,2,1}$  ( $g = 15$ ), leading to the total statistical weight  $g_{n=3} = g_{3s} + g_{3p} + g_{3d} = 36$ .

The procedure can be continued to get all excited states coming from the interaction of the core electron with the optical electron. By comparing the total statistical weight coming from  $n = 2$  and  $n = 3$  we can deduce that the statistical weight of helium follows the relation

$$g = 4n^2$$

with respect to the principal quantum number.

Concerning the energy of levels, to a first approximation we can use an *hydrogenic* formula, inserting the helium ionization potential  $I_{\text{He}}$  in place of the corresponding one of the hydrogen atom

$$E_n = I_{\text{He}} - \frac{I_H}{n^2}$$



neglecting the splitting between singlet and triplet states due to spin-orbit coupling. Note also that the *He* ground state has a statistical weight  $g = 1$ .

### A.2.2 Oxygen

We have already studied the spectroscopic terms coming from the different interactions occurring in the  $p^4$  configuration. Now we want to study the interaction of the most stable atomic oxygen core (i.e., the  $^4S_{3/2}$  state  $L_{\text{core}} = 0$ ,  $S_{\text{core}} = 3/2$ ) with the optical electron jumping on the excited states with  $n \geq 3$ . The stable core derives from the elimination of one electron from the  $p^4$  to obtain the  $p^3$  configuration.

Combining the core and an electron with  $n = 4$ , thus with  $\ell = 0, \dots, n - 1 = 0, 1, 2, 3$ , the following atomic terms can be derived

$\ell$	$s$	$L$	$S$	$J$	Terms	$g$
0	1/2	0	{2,1}	{2,1}	$^5S_2, ^3S_1$	8
1	1/2	1	2	{3,2,1}	$^5P_{3,2,1}$	15
1	1/2	1	1	{2,1,0}	$^3P_{2,1,0}$	9
2	1/2	2	2	{4,3,2,1,0}	$^5D_{4,3,2,1,0}$	25
2	1/2	2	1	{3,2,1}	$^3D_{3,2,1}$	15
3	1/2	3	2	{5,4,3,2,1}	$^5F_{5,4,3,2,1}$	35
3	1/2	3	1	{4,3,2}	$^3F_{4,3,2}$	21

giving a total statistical weight  $g = 128$ . For  $n = 3$ , only the contribution of state with  $\ell = 0 - 2$  must be considered, giving a total statistical weight  $g = 72$ .

We can deduce that the statistical weight for states obtained by the interaction of the  $^4S$  core with the optical electron with  $n > 2$  is reproduced by the general formula

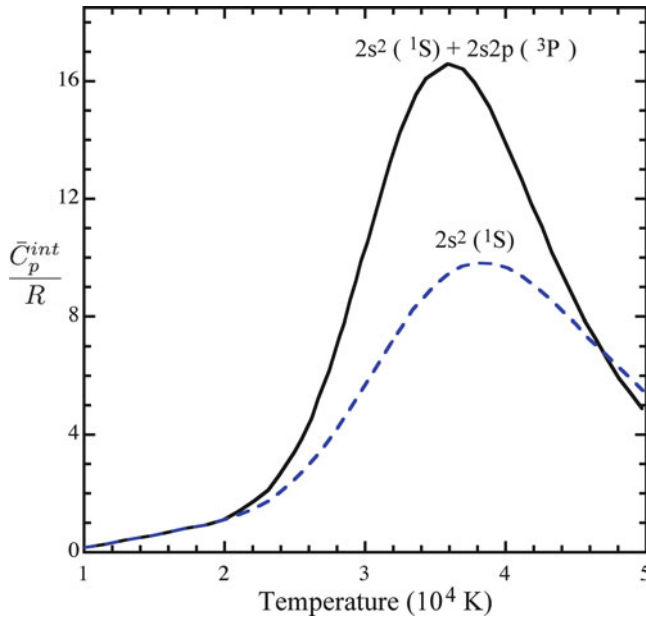
$$g_n = 8n^2.$$

Again, we can approximate the energy of the excited states through an hydrogenic form

$$E_n = I_O - \frac{I_H}{n^2}.$$

We must note that other sequences can arise forming electronically excited states of oxygen atoms from different core configurations. In fact, keeping in mind that low-lying excited states of oxygen are formed from different  $L - S$  of the core electrons as  $^1S$  or  $^1D$  states. The new series are obtained repeating the previous procedure to each core configuration, obtaining plenty of the different levels. The corresponding energy can be calculated by the hydrogenic formula

$$E_n^* = I_O - \frac{I_H}{n^2} + E_{\text{core}},$$



**Fig. A.3** Reduced internal specific heat of  $C^+$  as a function of temperature: comparison between calculations including levels having core  $2s^2 ({}^1S)$  and  $2s^2 ({}^1S) + 2s2p({}^3P)$

where  $E_{\text{core}}$  is the energy of the excited core configuration with respect to the ground state. The energy of the states of these series rapidly overcomes the ionization potential of the ground  $I_O$  forming the autoionizing states of the atom.

These states, while having energies above the ionization potential, are in same case considered, especially in the astrophysical literature. In this context, it is interesting to analyze their effects on the partition function and on thermodynamic properties. In Fig. A.3, we can see the effects on the internal specific heat of  $C^+$  of the autoionizing states coming from  $2s2p ({}^3P)$  core.

As a general rule, we can calculate the statistical weight of excited states obtained from the interaction of a given core with the excited electron using the general formula

$$g_n = 2g_{\text{core}}n^2,$$

where  $g_{\text{core}}$  is the statistical weight of the relative core configuration. Keeping in mind that the electronic configuration of the helium core is a  ${}^2S$  state we have  $g_{\text{core}} = 2$ , while for  ${}^4S$  core of oxygen  $g_{\text{core}} = 4$ .

### A.3 Beyond the Hydrogenoid Approximation

The available database for observed atomic electronic energy levels, as Moore (1949) and NIST tables (Chase Jr. 1998; NIST 2009), miss most of the predicted electronic levels, especially for higher quantum numbers.

In this section, we present a useful semi-empirical procedure which, applying a simplified formula to available, experimental or calculated, electronic levels, allows to complete, interpolating and/or extrapolating, the level series. We apply this method to estimate level energies of neutral carbon atom (see (Capitelli and Molinari 1970) for the nitrogen atom). The structure of the ground state is very complex, due to the presence of a few of low-lying states resulting from different L–S coupling:

Configuration	Terms
$2s^2 2p^2$	$^1S, ^3P, ^1D$
$2s^1 2p^3$	$^5S, ^3S, ^3P, ^1P, ^3D, ^1D$
$2p^4$	$^1S, ^3P, ^1D$

The first three states results from rearrangement of the spin of the  $p$  electrons, while the others are obtained from different rearrangements of the angular momenta.

The first step of the procedure is to determine the energy of the ground state configuration. If one of these terms has not been observed, it can be derived through extrapolation from energy levels of isoelectronic species. Practically, for carbon, the term  $2p^4(^1S)$  is missing. We have to consider the energies of  $N^+$ ,  $O^{+2}$  and  $F^{+3}$ , corresponding to the same term, and, relating these energies to the atomic number  $Z$ , we extrapolate to obtain the corresponding value for  $Z = 6$  (carbon).

The excited states come from the excitation of one electron toward higher values of the principal quantum numbers ( $n > 2$ ) giving for carbon atoms

$$\begin{aligned}
 &2s^2 2p(^2P)n\ell \\
 &2s 2p^2(^4P)n\ell \\
 &2s 2p^2(^2D)n\ell \\
 &2s 2p^2(^2S)n\ell \\
 &2s 2p^2(^2P)n\ell \\
 &2p^3(^4S)n\ell,
 \end{aligned}$$

where each series arises from the interaction of different atomic cores,  $2s^2 2p(^2P)$ ,  $2s 2p^2(^4P)$ ,  $\dots$ , with the excited electron, where  $x = s, p, d, \dots$ . It should be noted that in the previous section we have discussed only the excited states coming from the interaction of the more stable core,  $2s^2 2p(^2P)$ , with the excited electron. In this case, for  $\ell = s$ , there are two spectroscopic terms:  $^3P$  ( $L = 1, S = 1$ ), and  $^1P$  ( $L = 1, S = 0$ ). NIST's tables (NIST 2009) report observed levels up to

$n = 10$  for the former and  $n = 14$  (missing values  $n = 11, 12$ ) for the latter. To extrapolate to higher principal quantum numbers, the following Ritz–Rydberg series can be used:

$$E_n = I - \frac{I_H(z+1)^2}{\left(n + A + \frac{B}{n^2}\right)^2}, \quad (\text{A.1})$$

where  $z$  is the charge of the species and  $A, B$  are adjustable parameters. The ionization energy  $I$  is related to the specific core configuration. It is calculated as the sum of the ionization energy from the ground state and the energy of the excited state of the successive ion in the corresponding electronic state. For example, if we consider  $C$  in the  $2s2p^2(^4P)n\ell$  series,  $I$  is the sum of the ionization potential of  $C$  from the ground state (11.260 eV) and the energy of the  $C^+$  in the excited state  $2s2p^2(^4P)$  (5.336 eV).

The constants  $A$  and  $B$  can be determined when at least two observed levels are available. If we have only two levels, it is straightforward to calculate  $A$  and  $B$  by solving a system of two equations in two unknowns. If more than two levels are available, the two parameters are calculated by a *best fit* procedure. When only one observed energy level is known in a series, (A.1) cannot be used and the following formula with a single adjustable parameter should be applied:

$$E_n = I - \frac{I_H(z+1)^2}{(n+A)^2} \quad (\text{A.2})$$

obtained from (A.1) considering  $B = 0$ .

In some cases, as for  $2s2p^2(^2P)n\ell$  for  $n > 4$  and  $\ell = g$ , no level has been observed. As an example, to obtain the energy level of the terms corresponding to  $5g$ , we relate the energy levels ( $5s, 5p, 5d, 5f$ ) as a function of the azimuthal quantum number  $\ell (= 0 - 3)$ , and extrapolate to  $\ell = 4$  (see also (Capitelli and Molinari 1970)).

This method has been applied up to  $n = 20$  and  $\ell = 19$ , with the exception of those series where no observed energies are present. For  $n > 20$ , we assume an hydrogen-like behavior and use the following formulas:

$$E_n = I - \frac{I_H(z+1)^2}{n^2}. \quad (\text{A.3})$$

At fixed  $n$  and for each series, the sum over the statistical weights of all the corresponding predicted spectroscopic terms for different  $\ell$  is equal to

$$g_n = 2n^2 g_{\text{core}} \quad (\text{A.4})$$

and for  $n > 20$  we apply this last equation to determine the total statistical weight. This method is more accurate than the hydrogenic approximation (see Sect. A.2) and has been extensively used in the calculation of thermodynamic properties of thermal plasmas.

## A.4 Electronic Terms of Diatomic Molecules

Analogously to the case of atomic systems, also molecular electronic states are classified through the value of quantum numbers associated with total orbital and spin angular momenta and the information is condensed in the corresponding *molecular term symbol*.

In diatoms the electric field has an axial symmetry, with respect to the internuclear axis and therefore the Hamiltonian commutes with the operator corresponding to the axial projection of orbital angular momentum, corresponding to the quantum number  $\Lambda$ . Capital greek letters ( $\Sigma$ ,  $\Pi$ ,  $\Delta$ ,  $\Phi$ , ...) are used for classification of molecular terms depending on the value assumed by  $\Lambda$  in the sequence (0, 1, 2, 3, ...). Moreover, each electronic term is characterized by the total spin  $S$ , with multiplicity  $(2S + 1)$  originating *doublets* ( $2S + 1 = 2$ ), *triplets* ( $2S + 1 = 3$ ), *quartets* ( $2S + 1 = 4$ ), ..., as seen for atoms. The general term symbol assumes the form:  $(^{2S+1})\Lambda$ .

In the case of diatomic molecules, the term symbol also retains information about the parity of the electronic wavefunction with respect to some symmetry operations. More in detail, the reflection about a plane containing the internuclear axis returns a state with the same energy but with opposite sign of the projection of the orbital angular momentum, thus leading to the conclusion that all terms with  $\Lambda \neq 0$  are doubly degenerate. However for  $\Sigma$  states ( $\Lambda = 0$ ), which are nondegenerate, the parity is usually specified adding the sign plus or minus as superscript to the term symbol for even or odd states, i.e.  $(^{2S+1})\Sigma^{+/-}$ .

Finally in the case of homonuclear diatomic molecules, a new symmetry arises due to the inversion center bisecting the internuclear axis. In this case, the subscripts  $g$  and  $u$  are used ( $(^{2S+1})\Lambda_{g/u}$ ) for even (*gerade*) and odd (*ungerade*), respectively.

In the following, the *Wigner-Withmer rules* for the construction of molecular electronic terms for diatomic molecules arising from the interaction of atoms in given electronic states are illustrated.

The  $\Lambda$  value is determined as the modulus of the algebraic sum of axial projections of orbital angular momenta of atoms, i.e.,  $\Lambda = |M_{L_1} + M_{L_2}|$ , assuming values in the series,  $M_{L_1} = L_1, L_1 - 1, \dots, 0, \dots, -L_1$  and  $L_2 = L_2, L_2 - 1, \dots, 0, \dots, -L_2$ . If  $L_1 \geq L_2$  it can be demonstrated that, accounting for double degeneracy of terms with  $\Lambda \neq 0$ ,  $(2L_2 + 1)(L_1 + 1)$  terms arise with  $\Lambda$  assuming values from 0 to  $L_1 + L_2$ . The number of molecular terms for each symmetry, given the orbital angular momenta of atoms, is given in Table A.2.

The atomic spin  $S_1$  and  $S_2$  vectorially sum in the total spin  $S$ , assuming values in the series  $S_1 + S_2, S_1 + S_2 - 1, \dots, |S_1 - S_2|$ .

**Table A.2** Number of molecular terms per symmetry in diatomic molecules, for given orbital angular momenta of atoms

Number of terms	$\Lambda$
1	$L_1 + L_2$
2	$L_1 + L_2 - 1$
3	$L_1 + L_2 - 2$
...	...
$(2L_2+1)$	$L_1 - L_2$
$(2L_2+1)$	$L_1 - L_2 - 1$
...	...
$(2L_2+1)$	0

### A.4.1 $H_2$ Molecule

(a) – *Molecular states arising from two atoms in the ground state*

The ground state of the hydrogen atom is a  $^2S$  state therefore  $S = 1/2$  and  $L = 0$ . Using the combination rules, we have

$$\begin{aligned} \Lambda &= L_1 + L_2 = 0 && \Rightarrow \Sigma \\ S &= S_1 + S_2, |S_1 - S_2| = 1, 0 && \Rightarrow \text{triplet and singlet} \end{aligned}$$

Therefore, two molecular states arise:  $^1\Sigma$  and  $^3\Sigma$ .

To characterize better the symmetry of the states, we must know the parity of the wave functions. For the hydrogen molecule, we can use either Heitler–London or molecular orbital (MO) wave functions. By using Heitler–London wave functions we must remind that the spatial part of these wave functions for the two states are written (neglecting the normalization factor) as

$$\begin{aligned} ^1\Sigma & \quad 1s_a(1)1s_b(2) + 1s_a(2)1s_b(1) \\ ^3\Sigma & \quad 1s_a(1)1s_b(2) - 1s_a(2)1s_b(1), \end{aligned}$$

where  $1s_a(1)$  represents an hydrogen wave function centered on the atom  $a$  describing electron 1. On the other hand,  $1s_b(2)$  represents an hydrogen wave function centered on the atom  $b$  describing electron 2. The other terms mix the coordinates of the two electrons. By applying the symmetry operations generated by inversion through the molecule center and by reflection through a plane containing the internuclear axis to the first wave function one finds its invariants so that in the molecular state should appear the  $g$  and  $+$  characters, i.e., the singlet state should be better written as  $^1\Sigma_g^+$ . The same operators applied to the triplet state should add the characters  $u$  and  $+$  to the wavefunction, i.e., the triplet state should be written as  $^3\Sigma_u^+$ . To conclude we have written the first two molecular states of molecular hydrogen, the ground  $X^1\Sigma_g^+$  and the first excited state  $b^3\Sigma_u^+$ . The triplet state is repulsive so that it does not enter in the electronic partition function. However, the repulsive state, which plays an important role on the transport properties and on the chemical kinetics of a plasma, should be taken into account also in thermodynamics

when considering real gas effects, i.e., the virial coefficients (see Chap. 7). The statistical weight of the  $\Sigma$  states is equal to the spin multiplicity, which is the number of total wave functions (space and spin) describing the state. According to the Pauli exclusion principle, the total wave function (space and spin) must be antisymmetric under the exchange of every couple of electrons (Capitelli et al. 2011b; Pauling and Wilson 1985). Keeping in mind the spin wave-functions  $\alpha$  and  $\beta$  we can write the following (a part the normalization factor) wave functions for the two electron spin system

$$\sigma_{\text{singlet}} = \alpha(1)\beta(2) - \alpha(2)\beta(1)$$

$$\sigma_{\text{triplet}} = \begin{cases} \alpha(1)\alpha(2) \\ \beta(1)\beta(2) \\ \alpha(1)\beta(2) + \alpha(2)\beta(1). \end{cases}$$

To keep antisymmetric the total wavefunction we must couple symmetric space part with the antisymmetric spin part and vice versa. Therefore for the first two states of hydrogen molecule, we obtain

$${}^1\Sigma_g^+ \propto [1s_a(1)1s_b(2) + 1s_a(2)1s_b(1)][\alpha(1)\beta(2) - \alpha(2)\beta(1)]$$

$${}^3\Sigma_u^+ \propto [1s_a(1)1s_b(2) - 1s_a(2)1s_b(1)] \cdot \begin{cases} \alpha(1)\alpha(2) \\ \beta(1)\beta(2) \\ \alpha(1)\beta(2) + \alpha(2)\beta(1) \end{cases}$$

To get the energies of the different states, we must apply the Hamiltonian operator of  $H_2$  molecule to the relevant wave functions. These energies depend on the internuclear distance resulting in the potential energy curves. Nowadays, molecular states are obtained by quantum chemistry approaches, i.e., *Harthree–Fock* (HF), *configuration interaction* (CI) and high-level post-HF methods (see (Szabo and Ostlund 1996)).

#### (b) – Molecular states arising from excited atoms

Many other bound states can enter in the electronic partition function of molecular hydrogen. As an example from the interaction between  $H(1s) + H(2s, 2p)$  atomic states, we can obtain the following 12 (bound and unbound) molecular states:  ${}^{1,3}\Sigma_{g,u}^+$  (from  $1s + 2s$ ) and  ${}^{1,3}\Sigma_{g,u}^+, {}^{1,3}\Pi_{g,u}$  (from  $1s + 2p$ ), while in the interaction between  $H(1s) + H(3s, 3p, 3d)$  we obtain 24 molecular states (Capitelli et al. 1974) and so on. Most of these states have been inserted in the results of Fig. 5.4, which in particular includes a series of excited states with a total multiplicity of 129 and energy ranging from 91700 to 123488.0  $\text{cm}^{-1}$  (see (Pagano et al. 2008) for details). The potential curves of the most important electronic states of  $H_2$ ,  $H_2^+$  and  $H_2^-$  are reported in Fig. A.4 adapted from (Sharp 1970).

Note also that other excited states can be constructed from the interaction between  $H(2s)$  and  $H(ns, np, \dots)$  with  $n > 1$ . These states are characterized by very large excitation energies and many terms are purely repulsive (Celiberto et al. 1998).

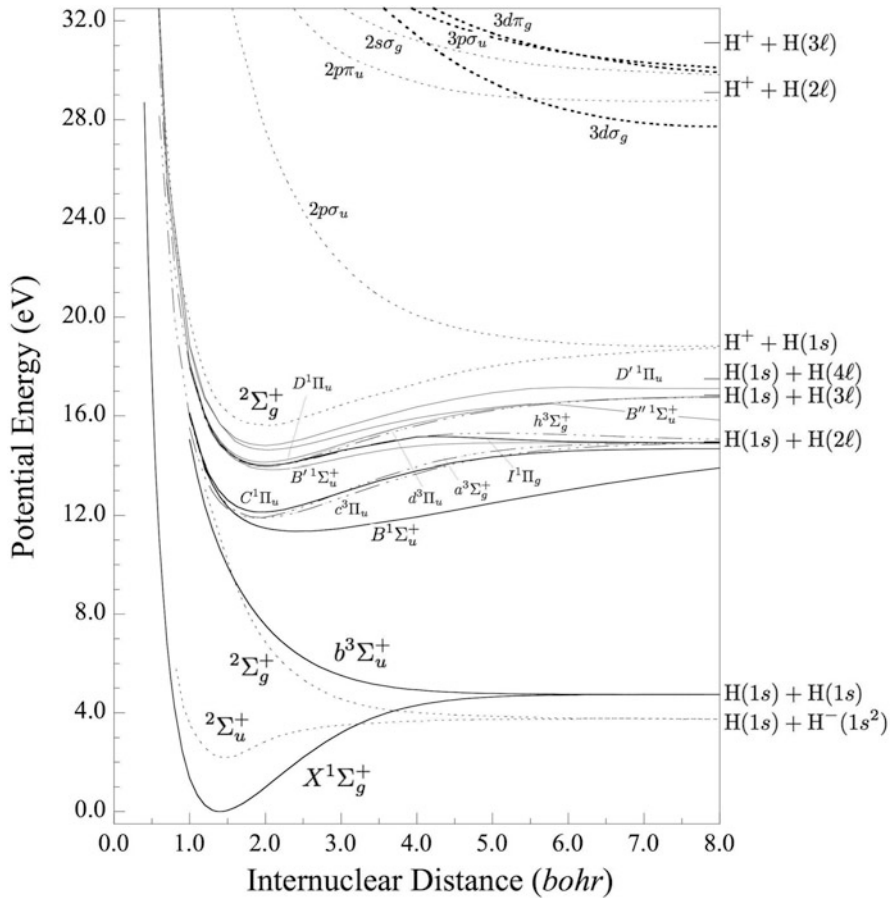


Fig. A.4 Energy diagram for  $H_2$  molecule and its molecular ions

### A.4.2 $N_2$ Molecule

(a) – Molecular states arising from two atoms in the ground state

The ground state of the nitrogen atom is  $^4S$ ; therefore,  $S = 3/2$  and  $L = 0$ . Using the combination rules, we have

$$\begin{aligned} A &= L_1 + L_2 = 0 && \Rightarrow \Sigma \\ S &= S_1 + S_2, \dots |S_1 - S_2| = 3, 2, 1, 0 && \Rightarrow \text{septet, quintet,} \\ &&& \text{triplet and singlet (ground).} \end{aligned}$$

In the interaction, we form four  $\Sigma$  states ( $^1\Sigma$ ,  $^3\Sigma$ ,  $^5\Sigma$ ,  $^7\Sigma$ ). Considering the interaction of two identical atoms the *gerade/ungerade* symmetry should be



taken into account and being the two atoms in identical quantum states there are restrictions on the number of terms, in particular if  $S$  is even  $N_g^+ = N_u^- + 1 = L + 1$ , while for  $S$  odd  $N_u^+ = N_g^- + 1 = L + 1$ . Therefore, the different molecular wave functions show the following symmetries:  $^1\Sigma_g^+$ ,  $^3\Sigma_u^+$ ,  $^5\Sigma_g^+$ ,  $^7\Sigma_u^+$ . The increase of spin multiplicity gives more antibonding character to the potential curves. So the singlet state in which all the spins are paired is strongly bounded, while the septet state, in which all spins are unpaired, is the most repulsive state. It should be noted that the triplet state is bounded and represents a metastable state playing an important role in the kinetics of nitrogen plasmas (Colonna and Capitelli 2001a).

(b) – *Molecular states arising from one atom in the ground state and one atom in the excited  $^2D$  state*

The excited  $^2D$  state of the nitrogen atom is characterized by  $L_1 = 2$  and  $S_1 = 1/2$ , and the interaction with the  $^4S$  ground state,  $L_2 = 0$  and  $S_2 = 3/2$ , leads to

$$\begin{aligned} \Lambda &= L_1 + L_2, \dots, |L_1 - L_2| = 2, 1, 0 & \Rightarrow \Delta, \Pi \text{ and } \Sigma \\ S &= S_1 + S_2, \dots, |S_1 - S_2| = 2, 1 & \Rightarrow \text{quintet and triplet} \end{aligned}$$

Therefore, we obtain the following states:  $^3\Sigma$ ,  $^3\Pi$ ,  $^3\Delta$ ,  $^5\Sigma$ ,  $^5\Pi$ ,  $^5\Delta$ . In this case considering an homonuclear diatomic system, i.e. identical atoms, states with *gerade/ungerade* parity arise and, being the atoms in different quantum states, all the states exist. Therefore in the interaction  $^4S+^2D$  12 states arise:  $^3\Sigma_{g,u}$ ,  $^3\Pi_{g,u}$ ,  $^3\Delta_{g,u}$ ,  $^5\Sigma_{g,u}$ ,  $^5\Pi_{g,u}$ ,  $^5\Delta_{g,u}$ . It can be demonstrated (Landau and Lifshitz 1981) that, concerning the parity of  $\Sigma$  states,  $(2L_2 + 1) \Sigma^+$  terms and  $L_2 \Sigma^-$  terms are found when the factor  $(-1)^{L_1+L_2} P_1 P_2 = 1$  and the opposite is true when the factor is equal to  $-1$ , being  $P_i$  the parity of the state of  $i$ -th atom. In this case we have  $^3\Sigma_{g,u}^+$ ,  $^3\Pi_{g,u}$ ,  $^3\Delta_{g,u}$ ,  $^5\Sigma_{g,u}^+$ ,  $^5\Pi_{g,u}$ ,  $^5\Delta_{g,u}$ . Some of them are repulsive and do not enter in the partition function.

(c) – *Molecular states arising from one atoms in the ground state and one atom in the excited  $^2P$  state*

The excited  $^2P$  state of the nitrogen atom is characterized by  $L_1 = 1$  and  $S_1 = 1/2$ , and the interaction with the  $^4S$  ground state,  $L_2 = 0$  and  $S_2 = 3/2$ , leads to

$$\begin{aligned} \Lambda &= L_1 + L_2, \dots, |L_1 - L_2| = 1, 0 & \Rightarrow \Pi \text{ and } \Sigma \\ S &= S_1 + S_2, \dots, |S_1 - S_2| = 2, 1 & \Rightarrow \text{quintet and triplet.} \end{aligned}$$

The following states arise:  $^{3,5}\Sigma_{g,u}^-$ ,  $^{3,5}\Pi_{g,u}$ .

(d) – *Molecular states arising from one atom in the  $^2D$  state and one atom in the excited  $^2P$  state*

Let us consider the interaction between  $N(^2D)$ , with  $L_1 = 2$  and  $S_1 = 1/2$ , and  $N(^2P)$ , with  $L_2 = 1$  and  $S_2 = 1/2$ .

$$\begin{aligned} \Lambda &= L_1 + L_2, \dots, |L_1 - L_2| = 3, 2, 1, 0 &\Rightarrow \Phi, \Delta, \Pi \text{ and } \Sigma \\ S &= S_1 + S_2, \dots, |S_1 - S_2| = 1, 0 &\Rightarrow \text{triplet and singlet.} \end{aligned}$$

In this case, the number of terms for each symmetry is higher than 1, in fact following Table A.2 we have 3 states of symmetry  $^{1,3}\Sigma_{g,u}$ , 3 states of symmetry  $^{1,3}\Pi_{g,u}$ , 2 states of symmetry  $^{1,3}\Delta_{g,u}$  and 1 state of symmetry  $^{1,3}\Phi_{g,u}$ . Moreover being  $(-1)^{L_1+L_2} P_1 P_2 = -1$  two of the three  $\Sigma$  terms are odd (–) and only one is even (+). Therefore, the electronic terms are  $^{1,3}\Phi_{g,u}$ , (2) $^{1,3}\Delta_{g,u}$ , (3) $^{1,3}\Pi_{g,u}$ , (2) $^{1,3}\Sigma_{g,u}^-$  and  $^{1,3}\Sigma_{g,u}^+$ .

(e) – *Molecular states arising from two atoms in the  $^2D$  state*

The excited  $^2D$  state of the nitrogen atom, with  $L = 2$  and  $S = 1/2$ ,

$$\begin{aligned} \Lambda &= L_1 + L_2, \dots, |L_1 - L_2| = 4, 3, 2, 1, 0 &\Rightarrow \Gamma, \Phi, \Delta, \Pi \text{ and } \Sigma \\ S &= S_1 + S_2, \dots, |S_1 - S_2| = 1, 0 &\Rightarrow \text{triplet and singlet.} \end{aligned}$$

In the interaction, the number of states per symmetry is the following: five states  $^{1,3}\Sigma$ , four states  $^{1,3}\Pi$ , three states  $^{1,3}\Delta$ , two states  $^{1,3}\Phi$ , and one  $^{1,3}\Gamma$ . Being the interaction of two identical atoms in the identical quantum state, restrictions occurs on the number of state of *gerade/ungerade* symmetry, in particular

$\Lambda$ odd	$S$ even or odd	$N_g = N_u$
$\Lambda$ even	$S$ even	$N_g = N_u + 1$
$\Lambda$ even	$S$ odd	$N_u = N_g + 1$
$\Lambda = 0$	$S$ even	$N_g^+ = N_u^- + 1$
$\Lambda = 0$	$S$ odd	$N_u^+ = N_g^- + 1$

i.e.,  $^1\Gamma_g$ ,  $^3\Gamma_u$ ,  $^{1,3}\Phi_{g,u}$ , (2) $^1\Delta_g$ ,  $^1\Delta_u$ , (2) $^3\Delta_u$ ,  $^3\Delta_g$ , (2) $^{1,3}\Pi_{g,u}$ , (3) $^1\Sigma_g^+$ , (2) $^1\Sigma_u^-$ , (3) $^3\Sigma_u^+$ , (2) $^3\Sigma_g^-$ .

(f) – *Molecular states arising from two atoms in the  $^2P$  state*

The excited  $^2P$  state of the nitrogen atom, with  $S = 1/2$  and  $L = 1$ ,

$$\begin{aligned} \Lambda &= L_1 + L_2, \dots, |L_1 - L_2| = 2, 1, 0 &\Rightarrow \Delta, \Pi \text{ and } \Sigma \\ S &= S_1 + S_2, \dots, |S_1 - S_2| = 1, 0 &\Rightarrow \text{triplet and singlet.} \end{aligned}$$

The electronic terms are:  $^1\Delta_g$ ,  $^3\Delta_u$ ,  $^{1,3}\Pi_{g,u}$ , (2) $^1\Sigma_g^+$ ,  $^1\Sigma_u^-$ , (2) $^3\Sigma_u^+$ ,  $^3\Sigma_g^-$ .

### A.4.3 $N_2^+$ Molecule

(a) – Molecular states arising from  $N(^4S)$  and  $N^+(^3P)$

The nitrogen ion in the ground state ( $^3P$ ),  $L_1 = 1$  and  $S_1 = 1$ , interacting with the nitrogen atom in the ground state ( $^4S$ ),  $L_2 = 0$  and  $S_2 = 3/2$ , originates

$$\begin{aligned} \Lambda &= L_1 + L_2, \dots, |L_1 - L_2| = 1, 0 && \Rightarrow \Pi \text{ and } \Sigma \\ S &= S_1 + S_2, \dots, |S_1 - S_2| = 5/2, 3/2, 1/2 && \Rightarrow \text{sextet, quartet, and doublet} \end{aligned}$$

and considering the *gerade/ungerade* symmetry, being the atoms different, and the  $+/-$  parity  $((-1)^{L_1+L_2} P_1 P_2 = 1)$  we have  $^{2,4,6}\Sigma_{g,u}^+$ ,  $^{2,4,6}\Pi_{g,u}$ .

# Appendix B

## Tables of Partition Function of Atmospheric Species

In this appendix, we report tables of internal partition functions of species considered in the planetary atmospheres (Chap. 10).

For molecules, negative atomic ions and some positive atomic ions, as  $H^+$ ,  $He^{+2}$  and  $C^{+4}$ , internal partitions functions are independent of the pressure (see Tables B.1–B.7). For other species, self-consistent partition functions are reported with cutoff depending on the neutral or electron density as discussed in Chap. 8. For other species self-consistent partition functions in the relevant atmospheres are reported as a function of temperature for different pressures (see Tables B.8–B.39).

It should be noted that the atomic species reported in the *air* section are also present in the *Mars* section, because, due to the different composition of the two mixtures, the internal partition functions calculated using the self-consistent cutoff are slightly different.

### B.1 Partition Functions Independent of the Pressure

**Table B.1** Internal partition function as a function of temperature

$T$ (K)	$C_2$	$C_2^+$	$C_2^-$	$CN$	$CN^+$
100	19.4	84.2	40.3	74.2	269.9
200	41.8	167.8	80.3	147.8	537.9
300	78.5	251.9	120.4	221.4	806.7
400	134.7	337.9	160.7	295.2	1,079.4
500	209.2	427.9	201.8	369.7	1,361.8
600	299.8	523.5	244.3	445.7	1,659.7
700	405.2	625.9	288.7	524.1	1,977.3
800	524.4	735.7	335.3	605.5	2,317.7
900	657.0	853.4	384.6	690.4	2,682.9

(continued)

**Table B.1** (continued)

$T$ (K)	$C_2$	$C_2^+$	$C_2^-$	$CN$	$CN^+$
1,000	802.8	979.1	436.6	779.3	3,074.4
1,500	1,730.0	1,734.2	742.5	1,292.6	5,455.3
2,000	3,005.5	2,704.2	1,129.2	1,935.4	8,602.9
2,500	4,667.8	3,891.4	1,600.3	2,730.1	12,600.4
3,000	6,763.0	5,297.1	2,158.8	3,707.1	17,538.1
3,500	9,339.3	6,922.1	2,810.0	4,901.5	23,507.7
4,000	12,444.9	8,767.3	3,562.1	6,349.6	30,599.4
4,500	16,128.1	10,833.4	4,427.6	8,086.6	38,900.9
5,000	20,437.5	13,121.2	5,421.9	10,145.4	48,496.2
6,000	31,133.9	18,363.4	7,867.5	15,351.4	71,881.8
7,000	44,939.3	24,491.1	11,037.4	22,199.3	101,310.0
8,000	62,262.3	31,486.8	15,046.9	30,909.5	137,169.0
9,000	83,490.3	39,313.9	19,975.3	41,704.8	179,640.0
10,000	108,959.0	47,916.3	25,865.6	54,818.1	228,677.0
11,000	138,926.0	57,221.7	32,729.4	70,493.5	284,036.0
12,000	173,560.0	67,147.4	40,553.3	88,980.2	345,316.0
13,000	212,931.0	77,605.5	49,303.7	110,522.0	412,003.0
14,000	257,023.0	88,507.5	58,932.7	135,347.0	483,518.0
15,000	305,741.0	99,768.3	69,381.9	163,654.0	559,257.0
16,000	358,924.0	111,308.0	80,586.2	195,606.0	638,612.0
17,000	416,363.0	123,053.0	92,476.5	231,323.0	720,998.0
18,000	477,812.0	134,937.0	104,983.0	270,881.0	805,864.0
19,000	542,999.0	146,904.0	118,035.0	314,312.0	892,701.0
20,000	611,639.0	158,901.0	131,564.0	361,606.0	981,045.0
22,000	758,109.0	182,821.0	159,801.0	467,549.0	1,160,630.0
24,000	914,914.0	206,418.0	189,215.0	587,944.0	1,341,830.0
26,000	1,079,880.0	229,499.0	219,398.0	721,641.0	1,522,480.0
28,000	1,251,030.0	251,931.0	250,006.0	867,258.0	1,700,990.0
30,000	1,426,640.0	273,631.0	280,759.0	1,023,300.0	1,876,200.0
35,000	1,875,870.0	324,428.0	356,908.0	1,449,250.0	2,294,990.0
40,000	2,326,520.0	370,250.0	430,302.0	1,909,420.0	2,681,970.0
45,000	2,767,530.0	411,383.0	499,756.0	2,386,370.0	3,035,950.0
50,000	3,192,450.0	448,284.0	564,792.0	2,867,250.0	3,358,320.0

**Table B.2** Internal partition function as a function of temperature

$T$ (K)	$CN^-$	$CO$	$CO^+$	$CO_2$	$CO_2^+$
100	36.5	36.5	71.3	88.9	403.6
200	72.7	72.7	142.0	180.7	1,022.0
300	108.9	108.9	212.8	290.0	1,966.0
400	145.1	145.1	283.6	432.7	3,374.5
500	181.7	181.7	355.0	621.9	5,423.3
600	218.8	218.8	427.4	870.8	8,331.7
700	257.0	257.0	501.7	1,194.3	12,366.4
800	296.4	296.4	578.4	1,609.3	17,844.9
900	337.5	337.5	658.1	2,135.3	25,139.7
1,000	380.3	380.3	741.1	2,794.3	34,683.4
1,500	625.6	625.6	1,215.8	9,057.6	136,041.0
2,000	928.3	928.3	1,800.2	23,748.9	400,984.0
2,500	1,291.7	1,291.7	2,501.0	53,594.1	978,579.0
3,000	1,717.3	1,717.3	3,322.2	108,246.0	2,089,820.0
3,500	2,206.4	2,206.4	4,267.7	200,822.0	4,041,990.0
4,000	2,760.2	2,760.2	5,343.7	348,462.0	7,242,990.0
4,500	3,379.8	3,379.8	6,559.0	572,935.0	12,215,900.0
5,000	4,066.2	4,066.2	7,925.9	901,355.0	19,613,200.0
6,000	5,644.2	5,644.7	11,180.2	2,010,980.0	45,025,600.0
7,000	7,503.8	7,508.3	15,266.1	4,042,960.0	91,818,700.0
8,000	9,655.5	9,677.9	20,378.5	7,538,410.0	171,203,000.0
9,000	12,110.6	12,192.9	26,732.5	13,289,000.0	297,463,000.0
10,000	14,881.4	15,122.0	34,548.8	22,428,500.0	487,950,000.0
11,000	17,980.5	18,573.5	44,037.7	36,529,500.0	762,868,000.0
12,000	21,420.7	22,700.7	55,386.3	57,695,300.0	1,144,870,000.0
13,000	25,213.7	27,701.0	68,747.5	88,632,800.0	1,658,500,000.0
14,000	29,370.0	33,810.0	84,233.8	132,700,000.0	2,329,600,000.0
15,000	33,897.5	41,291.0	101,915.0	193,921,000.0	3,184,620,000.0
16,000	38,801.5	50,422.5	121,821.0	276,974,000.0	4,249,980,000.0
17,000	44,084.1	61,486.4	143,941.0	387,151,000.0	5,551,490,000.0
18,000	49,744.1	74,756.7	168,233.0	530,289,000.0	7,113,780,000.0
19,000	55,777.4	90,490.2	194,628.0	712,691,000.0	8,959,920,000.0
20,000	62,176.7	108,920.0	223,033.0	941,037,000.0	11,111,000,000.0
22,000	76,031.0	154,658.0	285,432.0	1,563,550,000.0	16,401,400,000.0
24,000	91,202.0	213,232.0	354,450.0	2,455,030,000.0	23,107,400,000.0
26,000	107,559.0	285,412.0	429,037.0	3,672,620,000.0	31,312,000,000.0
28,000	124,959.0	371,519.0	508,158.0	5,270,860,000.0	41,060,200,000.0
30,000	143,253.0	471,506.0	590,843.0	7,299,850,000.0	52,363,000,000.0
35,000	191,954.0	779,484.0	807,644.0	14,530,900,000.0	87,241,400,000.0
40,000	243,299.0	1,161,730.0	1,030,590.0	25,217,400,000.0	130,814,000,000.0
45,000	295,677.0	1,605,250.0	1,252,370.0	39,601,000,000.0	181,761,000,000.0
50,000	347,918.0	2,096,840.0	1,468,410.0	57,697,300,000.0	238,617,000,000.0

**Table B.3** Internal partition function as a function of temperature

$T$ (K)	$CO_2^-$	$C_2O$	$N_2$	$N_2^+$	$N_2^-$
100	506.7	515.7	17.6	36.5	83.2
200	1,436.5	1,168.2	35.1	72.7	,165.7
300	2,691.8	2,188.9	52.6	108.9	,248.3
400	4,328.1	3,752.3	70.1	145.1	,331.2
500	6,452.3	6,052.5	87.7	181.7	,415.1
600	9,197.3	9,325.7	105.5	218.8	,501.0
700	12,714.7	13,858.6	123.6	256.8	,589.9
800	17,173.6	19,994.0	142.3	296.1	,682.6
900	22,760.6	28,137.4	161.6	337.0	,779.6
1000	29,681.6	38,764.4	181.6	379.5	,881.5
1500	92,946.6	151,657.0	294.9	623.3	1,472.3
2000	232,951.0	452,222.0	433.1	926.5	2,209.4
2500	502,149.0	1,129,800.0	597.9	1,300.5	3,099.4
3000	971,748.0	2,489,200.0	790.0	1,760.2	4,145.6
3500	1,735,150.0	4,990,270.0	1,010.1	2,322.6	5,350.9
4000	2,911,330.0	9,290,960.0	1,258.6	3,005.2	6,717.8
4500	4,647,740.0	16,289,300.0	1,535.9	3,825.1	8,248.9
5000	7,122,000.0	27,158,900.0	1,842.5	4,798.9	9,946.8
6000	15,147,200.0	66,716,300.0	2,545.6	7,271.3	13,853.4
7000	28,996,500.0	143,419,000.0	3,372.4	10,547.6	18,459.9
8000	51,058,600.0	277,136,000.0	4,330.3	14,753.8	23,789.1
9000	83,959,900.0	490,902,000.0	5,432.2	20,018.5	29,863.5
10000	130,402,000.0	809,212,000.0	6,700.6	26,471.2	36,702.2
11000	193,006,000.0	1,256,250,000.0	8,170.8	34,236.0	44,318.8
12000	274,190,000.0	1,854,330,000.0	9,893.0	43,425.2	52,718.8
13000	376,077,000.0	2,622,810,000.0	11,932.4	54,132.2	61,898.5
14000	500,439,000.0	3,577,330,000.0	14,368.2	66,426.9	71,844.8
15000	648,679,000.0	4,729,550,000.0	17,290.2	80,353.2	82,535.6
16000	821,828,000.0	6,087,160,000.0	20,795.2	95,928.7	93,941.1
17000	1,020,570,000.0	7,654,090,000.0	24,983.0	113,146.0	106,025.0
18000	1,245,250,000.0	9,430,900,000.0	29,952.5	131,976.0	118,748.0
19000	1,495,960,000.0	11,415,200,000.0	35,798.2	152,370.0	132,065.0
20000	1,772,520,000.0	13,602,300,000.0	42,607.4	174,265.0	145,931.0
22000	2,401,460,000.0	18,556,000,000.0	59,417.9	222,241.0	175,130.0
24000	3,127,150,000.0	24,221,600,000.0	80,876.4	275,211.0	205,992.0
26000	3,942,870,000.0	30,515,500,000.0	107,290.0	332,421.0	238,187.0
28000	4,840,950,000.0	37,349,100,000.0	138,790.0	393,117.0	271,427.0
30000	5,813,280,000.0	44,635,100,000.0	175,354.0	456,588.0	305,458.0
35000	8,516,540,000.0	64,303,800,000.0	287,738.0	623,307.0	392,681.0
40000	11,517,600,000.0	85,209,100,000.0	426,328.0	795,278.0	481,109.0
45000	14,719,600,000.0	106,552,000,000.0	585,469.0	966,882.0	569,161.0
50000	18,046,800,000.0	127,785,000,000.0	759,530.0	1,134,550.0	655,843.0

**Table B.4** Internal partition function as a function of temperature

$T$ (K)	$N_2O$	$N_2O^+$	$NO_2$	$NO$	$NO^+$
100	166.3	389.8	861.9	168.5	35.3
200	341.9	1009.1	2446.7	335.6	70.3
300	563.9	1965.4	4609.0	502.9	105.3
400	866.5	3408.2	7469.7	670.8	140.3
500	1279.2	5518.6	11236.0	841.0	175.5
600	1833.7	8519.4	16161.2	1015.8	211.1
700	2566.9	12680.8	22533.7	1197.1	247.4
800	3521.4	18324.3	30676.2	1386.8	284.7
900	4746.1	25827.5	40946.7	1586.0	323.3
1000	6297.2	35628.0	53741.2	1795.6	363.3
1500	21450.5	139193.0	172308.0	3016.3	589.5
2000	57938.4	408191.0	438169.0	4546.1	865.1
2500	132975.0	989336.0	953588.0	6398.4	1193.9
3000	269926.0	2087540.0	1858040.0	8580.8	1577.3
3500	497077.0	3956690.0	3336340.0	11099.8	2016.6
4000	845383.0	6879780.0	5628370.0	13961.8	2512.7
4500	1345940.0	11144400.0	9039470.0	17173.4	3066.7
5000	2027870.0	17019800.0	13950700.0	20742.1	3679.5
6000	4036200.0	34488300.0	30232100.0	28988.3	5085.7
7000	7040820.0	60562400.0	59362700.0	38800.9	6741.1
8000	11186600.0	95725500.0	107886000.0	50330.7	8660.9
9000	16629800.0	139802000.0	184018000.0	63781.4	10871.9
10000	23561200.0	192163000.0	297492000.0	79395.7	13420.2
11000	32206900.0	251921000.0	459265000.0	97432.6	16378.0
12000	42814300.0	318074000.0	681110000.0	118143.0	19846.7
13000	55630600.0	389604000.0	975169000.0	141748.0	23955.6
14000	70883200.0	465541000.0	1353510000.0	168428.0	28857.4
15000	88765300.0	544992000.0	1827750000.0	198307.0	34720.3
16000	109427000.0	627158000.0	2408710000.0	231460.0	41719.2
17000	132970000.0	711337000.0	3106170000.0	267905.0	50027.6
18000	159453000.0	796919000.0	3928740000.0	307614.0	59809.7
19000	188888000.0	883384000.0	4883710000.0	350518.0	71214.7
20000	221254000.0	970288000.0	5977070000.0	396510.0	84372.4
22000	294528000.0	1143980000.0	8596430000.0	497205.0	116355.0
24000	378550000.0	1315680000.0	11809600000.0	608415.0	156345.0
26000	472339000.0	1483820000.0	15622300000.0	728686.0	204579.0
28000	574789000.0	1647380000.0	20025900000.0	856525.0	260988.0
30000	684761000.0	1805690000.0	25001400000.0	990496.0	325270.0
35000	985446000.0	2176650000.0	39754100000.0	1343790.0	517034.0
40000	1310990000.0	2511750000.0	57378000000.0	1710180.0	745158.0
45000	1649450000.0	2813070000.0	77304000000.0	2077580.0	999324.0
50000	1992130000.0	3083860000.0	99000100000.0	2438070.0	1270330.0



**Table B.5** Internal partition function as a function of temperature

$T$ (K)	$N_3$	$C_3$	$O_2$	$O_2^+$	$O_2^-$	$O_3$
100	219.0	180.2	73.4	83.4	121.5	649.8
200	520.3	798.6	146.4	166.1	242.6	1,849.7
300	878.2	2,035.8	219.6	248.9	365.8	3,536.3
400	1,332.7	4,037.9	293.7	332.1	495.4	5,900.8
500	1,925.8	6,972.8	369.9	416.5	635.5	9,217.9
600	2,700.6	11,044.5	449.8	503.2	788.6	13,806.1
700	3,704.8	16,493.6	534.2	593.3	956.0	20,028.8
800	4,992.8	23,594.9	623.9	687.5	1,138.6	28,300.3
900	6,626.0	32,656.5	719.4	786.5	1,337.0	39,090.5
1,000	8,674.0	44,017.7	820.9	890.8	1,551.4	52,929.1
1,500	28,221.0	149,384.0	1,426.6	1,499.2	2,872.2	190,983.0
2,000	74,308.0	381,187.0	2,207.2	2,264.1	4,622.2	526,364.0
2,500	168,295.0	818,489.0	3,179.2	3,193.0	6,819.4	1,238,070.0
3,000	340,902.0	1,566,530.0	4,362.5	4,291.2	9,482.5	2,675,800.0
3,500	633,930.0	2,768,050.0	5,779.1	5,563.0	12,633.0	5,506,510.0
4,000	1,101,980.0	4,621,180.0	7,452.3	7,013.3	16,295.7	10,836,500.0
4,500	1,814,090.0	7,402,970.0	9,405.7	8,647.5	20,499.8	20,243,300.0
5,000	2,855,290.0	11,497,700.0	11,663.6	10,472.4	25,277.0	35,707,800.0
6,000	6,351,960.0	25,892,500.0	17,194.2	14,732.6	36,674.1	93,931,100.0
7,000	12,628,900.0	54,286,400.0	24,249.0	19,901.3	50,681.7	204,051,000.0
8,000	23,012,100.0	107,075,000.0	33,019.3	26,139.0	67,365.5	382,505,000.0
9,000	39,087,700.0	199,666,000.0	43,654.5	33,648.5	86,643.2	641,412,000.0

10,000	62,645,100.0	353,459,000.0	56,242.5	42,650.8	108,310.0	988,037,000.0
11,000	95,603,500.0	596,628,000.0	70,804.9	53,358.5	132,080.0	1,425,220,000.0
12,000	139,932,000.0	964,670,000.0	87,303.6	65,954.3	157,630.0	1,952,240,000.0
13,000	197,572,000.0	1,500,680,000.0	105,653.0	80,578.1	184,630.0	2,565,730,000.0
14,000	270,372,000.0	2,255,340,000.0	125,733.0	97,320.8	212,761.0	3,260,510,000.0
15,000	360,034,000.0	3,286,590,000.0	147,403.0	116,225.0	241,734.0	4,030,260,000.0
16,000	468,072,000.0	4,659,120,000.0	170,511.0	137,291.0	271,289.0	4,868,080,000.0
17,000	595,788,000.0	6,443,490,000.0	194,902.0	160,478.0	301,203.0	5,766,840,000.0
18,000	744,257,000.0	8,715,230,000.0	220,422.0	185,717.0	331,282.0	6,719,450,000.0
19,000	914,323,000.0	11,553,700,000.0	246,924.0	212,914.0	361,365.0	7,719,080,000.0
20,000	1,106,610,000.0	15,040,800,000.0	274,269.0	241,957.0	391,319.0	8,759,260,000.0
22,000	1,559,250,000.0	24,295,000,000.0	330,983.0	305,081.0	450,420.0	10,937,500,000.0
24,000	2,103,130,000.0	37,141,500,000.0	389,654.0	374,034.0	507,938.0	13,211,400,000.0
26,000	2,736,580,000.0	54,214,700,000.0	449,531.0	447,748.0	563,471.0	15,545,600,000.0
28,000	3,455,920,000.0	76,091,400,000.0	510,008.0	525,213.0	616,795.0	17,911,400,000.0
30,000	4,256,040,000.0	103,272,000,000.0	570,600.0	605,510.0	667,801.0	20,286,200,000.0
35,000	6,568,700,000.0	196,892,000,000.0	720,293.0	813,593.0	785,151.0	26,154,800,000.0
40,000	9,243,160,000.0	329,859,000,000.0	864,612.0	1,024,820.0	888,765.0	31,796,600,000.0
45,000	12,177,400,000.0	502,778,000,000.0	1,001,620.0	1,232,930.0	980,153.0	37,125,100,000.0
50,000	15,282,600,000.0	713,774,000,000.0	1,130,530.0	1,434,160.0	1,060,940.0	42,108,400,000.0

**Table B.6** Internal partition function as a function of temperature

$T$ (K)	$O_3^-$	$C_2N$	$CNO$	$H_2$	$H_2^+$	$H_3^+$
100	650.0	263.8	449.0	2.3	5.1	0.6
200	1876.9	691.4	1123.2	2.5	7.0	1.5
300	3720.6	1411.2	2062.6	3.0	9.3	2.7
400	6483.7	2559.7	3396.9	3.5	11.7	4.0
500	10555.4	4308.1	5267.5	4.0	14.1	5.5
600	16392.6	6874.9	7840.0	4.6	16.7	7.1
700	24526.4	10529.7	11311.4	5.2	19.3	8.8
800	35569.9	15597.9	15912.9	5.8	22.0	10.7
900	50224.0	22465.0	21913.0	6.4	24.8	12.8
1000	69282.4	31581.9	29620.4	7.0	27.9	14.9
1500	265417.0	131936.0	107743.0	10.2	45.6	28.1
2000	750528.0	402924.0	302976.0	13.9	68.5	45.8
2500	1746700.0	1005810.0	716363.0	18.1	97.7	69.4
3000	3546140.0	2181850.0	1495660.0	22.9	134.3	100.9
3500	6503050.0	4268600.0	2844340.0	28.5	178.9	142.4
4000	11024400.0	7716250.0	5030530.0	34.9	231.8	197.0
4500	17565500.0	13104000.0	8395630.0	42.0	292.6	268.6
5000	26630000.0	21157000.0	13362200.0	50.2	360.7	362.1
6000	54598400.0	48987800.0	30230900.0	69.3	514.2	639.9
7000	99933900.0	100564000.0	60823500.0	92.7	684.0	1097.2
8000	168161000.0	188625000.0	111785000.0	120.3	862.4	1829.0
9000	264840000.0	329722000.0	191076000.0	151.9	1043.7	2961.7

1000	395048000.0	544469000.0	307699000.0	187.2	1223.7	4649.2
11000	562980000.0	857597000.0	471354000.0	225.7	1400.0	7063.5
12000	771731000.0	1297760000.0	692060000.0	267.0	1571.1	10381.5
13000	1023250000.0	1897150000.0	979789000.0	310.5	1736.6	14772.3
14000	1318400000.0	2690910000.0	1344130000.0	356.1	1896.9	20386.0
15000	1657090000.0	3716430000.0	1794030000.0	403.6	2053.1	27346.8
16000	2038460000.0	5012570000.0	2337530000.0	453.2	2206.9	35748.5
17000	2461030000.0	6618890000.0	2981700000.0	505.3	2360.3	45654.0
18000	2922860000.0	8574810000.0	3732460000.0	560.5	2515.6	57096.3
19000	3421680000.0	10918900000.0	4594590000.0	619.7	2675.5	70081.6
20000	3955020000.0	13688200000.0	5571690000.0	684.0	2842.6	84592.6
22000	5114870000.0	20640200000.0	7879780000.0	833.2	3208.5	118028.0
24000	6381510000.0	29678400000.0	10664500000.0	1019.9	3632.9	156940.0
26000	7734860000.0	41001300000.0	13919500000.0	1257.3	4131.7	200718.0
28000	9156490000.0	54753500000.0	17627200000.0	1558.0	4717.2	248690.0
30000	10630000000.0	71026700000.0	21762000000.0	1933.8	5397.4	300177.0
35000	14452100000.0	122907000000.0	33755100000.0	3262.1	7532.0	440139.0
40000	18343800000.0	190266000000.0	47668900000.0	5213.6	10265.3	589554.0
45000	22195100000.0	271594000000.0	62960700000.0	7808.0	13517.2	742174.0
50000	25939200000.0	364836000000.0	79155100000.0	11008.1	17181.2	893800.0

**Table B.7** Internal partition function as a function of temperature

$T$ (K)	$N^-$	$O^-$	$C^-$	$H^-$	$H^+$	$He^{+2}$	$C^{+4}$
100	6.5	4.2	4.000	1	1	1	1
200	7.4	4.6	4.000	1	1	1	1
300	7.9	4.9	4.000	1	1	1	1
400	8.1	5.1	4.000	1	1	1	1
500	8.3	5.2	4.000	1	1	1	1
600	8.4	5.3	4.000	1	1	1	1
700	8.5	5.4	4.000	1	1	1	1
800	8.5	5.5	4.000	1	1	1	1
900	8.6	5.5	4.000	1	1	1	1
1,000	8.6	5.6	4.000	1	1	1	1
1,500	8.7	5.7	4.001	1	1	1	1
2,000	8.8	5.8	4.008	1	1	1	1
2,500	8.9	5.8	4.033	1	1	1	1
3,000	8.9	5.8	4.086	1	1	1	1
3,500	8.9	5.9	4.169	1	1	1	1
4,000	9.0	5.9	4.282	1	1	1	1
4,500	9.1	5.9	4.419	1	1	1	1
5,000	9.1	6.0	4.576	1	1	1	1
6,000	9.3	6.0	4.927	1	1	1	1
7,000	9.5	6.1	5.302	1	1	1	1
8,000	9.7	6.3	5.680	1	1	1	1
9,000	9.9	6.4	6.048	1	1	1	1
10,000	10.1	6.5	6.400	1	1	1	1
11,000	10.2	6.7	6.732	1	1	1	1
12,000	10.4	6.8	7.044	1	1	1	1
13,000	10.6	7.0	7.336	1	1	1	1
14,000	10.7	7.1	7.608	1	1	1	1
15,000	10.9	7.2	7.862	1	1	1	1
16,000	11.0	7.4	8.098	1	1	1	1
17,000	11.1	7.5	8.319	1	1	1	1
18,000	11.3	7.6	8.525	1	1	1	1
19,000	11.4	7.7	8.718	1	1	1	1
20,000	11.5	7.9	8.899	1	1	1	1
22,000	11.7	8.1	9.227	1	1	1	1
24,000	11.9	8.3	9.517	1	1	1	1
26,000	12.0	8.4	9.776	1	1	1	1
28,000	12.2	8.6	10.007	1	1	1	1
30,000	12.3	8.8	10.214	1	1	1	1
35,000	12.6	9.1	10.651	1	1	1	1
40,000	12.8	9.3	10.999	1	1	1	1
45,000	13.0	9.6	11.282	1	1	1	1
50,000	13.2	9.8	11.517	1	1	1	1

## B.2 Selfconsistent Partition Functions of Atomic Species in Air Atmosphere

**Table B.8** Internal partition function of  $N$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	4.000	4.000	4.000	4.000	4.000
200	4.000	4.000	4.000	4.000	4.000
300	4.000	4.000	4.000	4.000	4.000
400	4.000	4.000	4.000	4.000	4.000
500	4.000	4.000	4.000	4.000	4.000
600	4.000	4.000	4.000	4.000	4.000
700	4.000	4.000	4.000	4.000	4.000
800	4.000	4.000	4.000	4.000	4.000
900	4.000	4.000	4.000	4.000	4.000
1000	4.000	4.000	4.000	4.000	4.000
1500	4.000	4.000	4.000	4.000	4.000
2000	4.000	4.000	4.000	4.000	4.000
2500	4.000	4.000	4.000	4.000	4.000
3000	4.001	4.001	4.001	4.001	4.001
3500	4.004	4.004	4.004	4.004	4.004
4000	4.010	4.010	4.010	4.010	4.010
4500	4.022	4.022	4.022	4.022	4.022
5000	4.041	4.041	4.041	4.041	4.041
6000	4.105	4.105	4.105	4.105	4.105
7000	4.208	4.208	4.208	4.208	4.208
8000	4.349	4.348	4.348	4.348	4.348
9000	4.524	4.523	4.522	4.522	4.522
10000	4.734	4.727	4.725	4.724	4.724
11000	4.990	4.961	4.952	4.949	4.948
12000	5.339	5.226	5.202	5.194	5.190
13000	5.886	5.538	5.474	5.454	5.448
14000	6.933	5.945	5.770	5.734	5.715
15000	8.969	6.531	6.117	6.022	5.996
16000	13.421	7.496	6.535	6.342	6.292
17000	20.994	9.189	7.055	6.698	6.583
18000	31.899	11.416	7.720	7.075	6.892
19000	51.586	15.737	8.649	7.522	7.224
20000	76.701	20.827	10.243	8.098	7.579
22000	157.071	40.912	14.091	9.476	8.366
24000	290.849	70.806	22.766	11.361	9.290
26000	533.113	115.802	33.449	14.015	10.400
28000	908.347	178.946	48.161	18.253	11.690
30000	1456.560	262.752	67.473	25.647	13.217
35000	3482.800	734.684	138.765	45.545	20.230
40000	6818.060	1330.920	295.223	73.924	30.919
45000	12485.900	2382.080	464.643	111.993	42.185
50000	19402.700	3873.690	693.668	157.473	56.773

**Table B.9** Internal partition function of  $N^+$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	3.250	3.250	3.250	3.250	3.250
200	5.065	5.065	5.065	5.065	5.065
300	6.045	6.045	6.045	6.045	6.045
400	6.641	6.641	6.641	6.641	6.641
500	7.039	7.039	7.039	7.039	7.039
600	7.323	7.323	7.323	7.323	7.323
700	7.536	7.536	7.536	7.536	7.536
800	7.700	7.700	7.700	7.700	7.700
900	7.832	7.832	7.832	7.832	7.832
1,000	7.939	7.939	7.939	7.939	7.939
1,500	8.274	8.274	8.274	8.274	8.274
2,000	8.448	8.448	8.448	8.448	8.448
2,500	8.555	8.555	8.555	8.555	8.555
3,000	8.630	8.630	8.630	8.630	8.630
3,500	8.688	8.688	8.688	8.688	8.688
4,000	8.738	8.738	8.738	8.738	8.738
4,500	8.786	8.786	8.786	8.786	8.786
5,000	8.835	8.835	8.835	8.835	8.835
6,000	8.938	8.938	8.938	8.938	8.938
7,000	9.054	9.054	9.054	9.054	9.054
8,000	9.180	9.180	9.180	9.180	9.180
9,000	9.314	9.314	9.314	9.314	9.314
10,000	9.453	9.453	9.453	9.453	9.453
11,000	9.596	9.596	9.596	9.596	9.596
12,000	9.740	9.740	9.740	9.740	9.740
13,000	9.886	9.886	9.886	9.886	9.886
14,000	10.031	10.031	10.031	10.031	10.031
15,000	10.177	10.177	10.177	10.177	10.177
16,000	10.322	10.321	10.321	10.321	10.321
17,000	10.467	10.466	10.466	10.466	10.466
18,000	10.613	10.610	10.610	10.610	10.610
19,000	10.763	10.755	10.753	10.753	10.753
20,000	10.923	10.901	10.897	10.896	10.896
22,000	11.304	11.207	11.187	11.183	11.182
24,000	11.917	11.559	11.492	11.475	11.472
26,000	13.176	12.029	11.826	11.778	11.766
28,000	16.075	12.742	12.222	12.102	12.071
30,000	22.390	14.048	12.731	12.459	12.391
35,000	69.675	23.333	15.019	13.638	13.342
40,000	225.137	51.463	21.169	15.674	14.601
45,000	640.863	111.804	35.915	19.772	16.371
50,000	1,478.330	258.378	60.511	26.071	18.844

**Table B.10** Internal partition function of  $N^{+2}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.325	2.325	2.325	2.325	2.325
200	3.141	3.141	3.141	3.141	3.141
300	3.733	3.733	3.733	3.733	3.733
400	4.136	4.136	4.136	4.136	4.136
500	4.422	4.422	4.422	4.422	4.422
600	4.633	4.633	4.633	4.633	4.633
700	4.795	4.795	4.795	4.795	4.795
800	4.923	4.923	4.923	4.923	4.923
900	5.027	5.027	5.027	5.027	5.027
1000	5.112	5.112	5.112	5.112	5.112
1500	5.384	5.384	5.384	5.384	5.384
2000	5.528	5.528	5.528	5.528	5.528
2500	5.618	5.618	5.618	5.618	5.618
3000	5.679	5.679	5.679	5.679	5.679
3500	5.723	5.723	5.723	5.723	5.723
4000	5.757	5.757	5.757	5.757	5.757
4500	5.783	5.783	5.783	5.783	5.783
5000	5.804	5.804	5.804	5.804	5.804
6000	5.836	5.836	5.836	5.836	5.836
7000	5.859	5.859	5.859	5.859	5.859
8000	5.877	5.877	5.877	5.877	5.877
9000	5.891	5.891	5.891	5.891	5.891
10000	5.904	5.904	5.904	5.904	5.904
11000	5.917	5.917	5.917	5.917	5.917
12000	5.930	5.930	5.930	5.930	5.930
13000	5.945	5.945	5.945	5.945	5.945
14000	5.963	5.963	5.963	5.963	5.963
15000	5.984	5.984	5.984	5.984	5.984
16000	6.008	6.008	6.008	6.008	6.008
17000	6.038	6.038	6.038	6.038	6.038
18000	6.071	6.071	6.071	6.071	6.071
19000	6.109	6.109	6.109	6.109	6.109
20000	6.152	6.152	6.152	6.152	6.152
22000	6.252	6.252	6.252	6.252	6.252
24000	6.371	6.371	6.371	6.371	6.371
26000	6.507	6.507	6.507	6.507	6.507
28000	6.660	6.659	6.659	6.659	6.659
30000	6.830	6.826	6.826	6.825	6.825
35000	7.379	7.308	7.299	7.298	7.298
40000	8.474	7.909	7.849	7.838	7.836
45000	12.158	8.787	8.494	8.442	8.429
50000	23.634	10.443	9.315	9.115	9.076



**Table B.11** Internal partition function of  $N^{+3}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.000	1.000	1.000	1.000	1.000
200	1.000	1.000	1.000	1.000	1.000
300	1.000	1.000	1.000	1.000	1.000
400	1.000	1.000	1.000	1.000	1.000
500	1.000	1.000	1.000	1.000	1.000
600	1.000	1.000	1.000	1.000	1.000
700	1.000	1.000	1.000	1.000	1.000
800	1.000	1.000	1.000	1.000	1.000
900	1.000	1.000	1.000	1.000	1.000
1,000	1.000	1.000	1.000	1.000	1.000
1,500	1.000	1.000	1.000	1.000	1.000
2,000	1.000	1.000	1.000	1.000	1.000
2,500	1.000	1.000	1.000	1.000	1.000
3,000	1.000	1.000	1.000	1.000	1.000
3,500	1.000	1.000	1.000	1.000	1.000
4,000	1.000	1.000	1.000	1.000	1.000
4,500	1.000	1.000	1.000	1.000	1.000
5,000	1.000	1.000	1.000	1.000	1.000
6,000	1.000	1.000	1.000	1.000	1.000
7,000	1.000	1.000	1.000	1.000	1.000
8,000	1.000	1.000	1.000	1.000	1.000
9,000	1.000	1.000	1.000	1.000	1.000
10,000	1.001	1.001	1.001	1.001	1.001
11,000	1.001	1.001	1.001	1.001	1.001
12,000	1.003	1.003	1.003	1.003	1.003
13,000	1.005	1.005	1.005	1.005	1.005
14,000	1.009	1.009	1.009	1.009	1.009
15,000	1.014	1.014	1.014	1.014	1.014
16,000	1.021	1.021	1.021	1.021	1.021
17,000	1.030	1.030	1.030	1.030	1.030
18,000	1.041	1.041	1.041	1.041	1.041
19,000	1.055	1.055	1.055	1.055	1.055
20,000	1.071	1.071	1.071	1.071	1.071
22,000	1.111	1.111	1.111	1.111	1.111
24,000	1.160	1.160	1.160	1.160	1.160
26,000	1.219	1.219	1.219	1.219	1.219
28,000	1.287	1.287	1.287	1.287	1.287
30,000	1.364	1.364	1.364	1.364	1.364
35,000	1.585	1.585	1.585	1.585	1.585
40,000	1.842	1.842	1.842	1.842	1.842
45,000	2.127	2.126	2.125	2.125	2.125
50,000	2.443	2.431	2.428	2.428	2.428

**Table B.12** Internal partition function of  $N^{+4}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.000	2.000	2.000	2.000	2.000
200	2.000	2.000	2.000	2.000	2.000
300	2.000	2.000	2.000	2.000	2.000
400	2.000	2.000	2.000	2.000	2.000
500	2.000	2.000	2.000	2.000	2.000
600	2.000	2.000	2.000	2.000	2.000
700	2.000	2.000	2.000	2.000	2.000
800	2.000	2.000	2.000	2.000	2.000
900	2.000	2.000	2.000	2.000	2.000
1000	2.000	2.000	2.000	2.000	2.000
1500	2.000	2.000	2.000	2.000	2.000
2000	2.000	2.000	2.000	2.000	2.000
2500	2.000	2.000	2.000	2.000	2.000
3000	2.000	2.000	2.000	2.000	2.000
3500	2.000	2.000	2.000	2.000	2.000
4000	2.000	2.000	2.000	2.000	2.000
4500	2.000	2.000	2.000	2.000	2.000
5000	2.000	2.000	2.000	2.000	2.000
6000	2.000	2.000	2.000	2.000	2.000
7000	2.000	2.000	2.000	2.000	2.000
8000	2.000	2.000	2.000	2.000	2.000
9000	2.000	2.000	2.000	2.000	2.000
10000	2.000	2.000	2.000	2.000	2.000
11000	2.000	2.000	2.000	2.000	2.000
12000	2.000	2.000	2.000	2.000	2.000
13000	2.001	2.001	2.001	2.001	2.001
14000	2.002	2.002	2.002	2.002	2.002
15000	2.003	2.003	2.003	2.003	2.003
16000	2.004	2.004	2.004	2.004	2.004
17000	2.007	2.007	2.007	2.007	2.007
18000	2.010	2.010	2.010	2.010	2.010
19000	2.013	2.013	2.013	2.013	2.013
20000	2.018	2.018	2.018	2.018	2.018
22000	2.031	2.031	2.031	2.031	2.031
24000	2.048	2.048	2.048	2.048	2.048
26000	2.069	2.069	2.069	2.069	2.069
28000	2.095	2.095	2.095	2.095	2.095
30000	2.126	2.126	2.126	2.126	2.126
35000	2.218	2.218	2.218	2.218	2.218
40000	2.330	2.330	2.330	2.330	2.330
45000	2.456	2.456	2.456	2.456	2.456
50000	2.590	2.589	2.589	2.589	2.589

**Table B.13** Internal partition function of *O* as a function of pressure and temperature

<i>T</i> (K)	<i>P</i> (bar)				
	10 <sup>-2</sup>	10 <sup>-1</sup>	1	10 <sup>1</sup>	10 <sup>2</sup>
100	5.346	5.346	5.346	5.346	5.346
200	6.156	6.156	6.156	6.156	6.156
300	6.741	6.741	6.741	6.741	6.741
400	7.140	7.140	7.140	7.140	7.140
500	7.423	7.423	7.423	7.423	7.423
600	7.633	7.633	7.633	7.633	7.633
700	7.794	7.794	7.794	7.794	7.794
800	7.922	7.922	7.922	7.922	7.922
900	8.025	8.025	8.025	8.025	8.025
1,000	8.110	8.110	8.110	8.110	8.110
1,500	8.382	8.382	8.382	8.382	8.382
2,000	8.527	8.527	8.527	8.527	8.527
2,500	8.617	8.617	8.617	8.617	8.617
3,000	8.680	8.680	8.680	8.680	8.680
3,500	8.729	8.729	8.729	8.729	8.729
4,000	8.772	8.772	8.772	8.772	8.772
4,500	8.813	8.813	8.813	8.813	8.813
5,000	8.855	8.855	8.855	8.855	8.855
6,000	8.947	8.947	8.947	8.947	8.947
7,000	9.051	9.051	9.051	9.051	9.051
8,000	9.166	9.166	9.166	9.166	9.166
9,000	9.292	9.290	9.290	9.290	9.290
10,000	9.431	9.422	9.420	9.419	9.418
11,000	9.600	9.566	9.555	9.552	9.550
12,000	9.847	9.723	9.697	9.689	9.685
13,000	10.268	9.913	9.848	9.828	9.821
14,000	11.127	10.179	10.011	9.975	9.957
15,000	12.813	10.643	10.207	10.121	10.097
16,000	16.469	11.295	10.456	10.289	10.244
17,000	22.474	12.571	10.776	10.479	10.380
18,000	30.786	14.197	11.197	10.678	10.530
19,000	45.510	17.378	11.839	10.926	10.693
20,000	63.599	20.980	12.903	11.263	10.870
22,000	119.269	34.913	15.408	12.084	11.272
24,000	208.037	54.645	21.150	13.208	11.755
26,000	364.340	83.334	27.833	14.731	12.332
28,000	599.187	122.388	36.825	17.664	13.016
30,000	933.420	172.861	48.349	21.854	13.845
35,000	2,113.170	450.162	89.066	33.184	18.615
40,000	3,975.420	780.587	177.202	48.770	23.441
45,000	7,060.660	1,351.720	267.024	68.198	29.256
50,000	10,708.900	2,142.700	393.197	92.912	36.572

**Table B.14** Internal partition function of  $O^+$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	7.000	7.000	7.000	7.000	7.000
200	7.000	7.000	7.000	7.000	7.000
300	7.000	7.000	7.000	7.000	7.000
400	7.000	7.000	7.000	7.000	7.000
500	7.000	7.000	7.000	7.000	7.000
600	7.000	7.000	7.000	7.000	7.000
700	7.000	7.000	7.000	7.000	7.000
800	7.000	7.000	7.000	7.000	7.000
900	7.000	7.000	7.000	7.000	7.000
1000	7.000	7.000	7.000	7.000	7.000
1500	7.000	7.000	7.000	7.000	7.000
2000	7.000	7.000	7.000	7.000	7.000
2500	7.000	7.000	7.000	7.000	7.000
3000	7.000	7.000	7.000	7.000	7.000
3500	7.000	7.000	7.000	7.000	7.000
4000	7.001	7.001	7.001	7.001	7.001
4500	7.003	7.003	7.003	7.003	7.003
5000	7.008	7.008	7.008	7.008	7.008
6000	7.030	7.030	7.030	7.030	7.030
7000	7.075	7.075	7.075	7.075	7.075
8000	7.152	7.152	7.152	7.152	7.152
9000	7.263	7.263	7.263	7.263	7.263
10000	7.409	7.409	7.409	7.409	7.409
11000	7.590	7.590	7.590	7.590	7.590
12000	7.801	7.801	7.801	7.801	7.801
13000	8.039	8.039	8.039	8.039	8.039
14000	8.300	8.300	8.300	8.300	8.300
15000	8.581	8.581	8.581	8.581	8.581
16000	8.877	8.877	8.877	8.877	8.877
17000	9.186	9.186	9.186	9.186	9.186
18000	9.505	9.505	9.505	9.505	9.505
19000	9.832	9.831	9.831	9.831	9.831
20000	10.164	10.163	10.163	10.163	10.163
22000	10.842	10.835	10.834	10.834	10.834
24000	11.545	11.516	11.509	11.508	11.508
26000	12.322	12.208	12.185	12.180	12.178
28000	13.334	12.934	12.864	12.846	12.841
30000	14.867	13.763	13.556	13.508	13.496
35000	25.683	17.316	15.519	15.188	15.116
40000	66.816	27.004	18.760	17.081	16.777
45000	189.602	50.258	25.666	19.850	18.613
50000	485.379	112.798	38.146	23.834	20.813

**Table B.15** Internal partition function of  $O^{+2}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.650	1.650	1.650	1.650	1.650
200	2.882	2.882	2.882	2.882	2.882
300	3.895	3.895	3.895	3.895	3.895
400	4.659	4.659	4.659	4.659	4.659
500	5.238	5.238	5.238	5.238	5.238
600	5.686	5.686	5.686	5.686	5.686
700	6.042	6.042	6.042	6.042	6.042
800	6.330	6.330	6.330	6.330	6.330
900	6.568	6.568	6.568	6.568	6.568
1,000	6.768	6.768	6.768	6.768	6.768
1,500	7.419	7.419	7.419	7.419	7.419
2,000	7.777	7.777	7.777	7.777	7.777
2,500	8.003	8.003	8.003	8.003	8.003
3,000	8.159	8.159	8.159	8.159	8.159
3,500	8.274	8.274	8.274	8.274	8.274
4,000	8.362	8.362	8.362	8.362	8.362
4,500	8.435	8.435	8.435	8.435	8.435
5,000	8.497	8.497	8.497	8.497	8.497
6,000	8.604	8.604	8.604	8.604	8.604
7,000	8.704	8.704	8.704	8.704	8.704
8,000	8.803	8.803	8.803	8.803	8.803
9,000	8.904	8.904	8.904	8.904	8.904
10,000	9.009	9.009	9.009	9.009	9.009
11,000	9.118	9.118	9.118	9.118	9.118
12,000	9.228	9.228	9.228	9.228	9.228
13,000	9.341	9.341	9.341	9.341	9.341
14,000	9.455	9.455	9.455	9.455	9.455
15,000	9.570	9.570	9.570	9.570	9.570
16,000	9.684	9.684	9.684	9.684	9.684
17,000	9.799	9.799	9.799	9.799	9.799
18,000	9.914	9.914	9.914	9.914	9.914
19,000	10.029	10.029	10.029	10.029	10.029
20,000	10.143	10.143	10.143	10.143	10.143
22,000	10.369	10.369	10.369	10.369	10.369
24,000	10.594	10.594	10.594	10.594	10.594
26,000	10.818	10.818	10.818	10.818	10.818
28,000	11.041	11.041	11.041	11.041	11.041
30,000	11.264	11.263	11.263	11.263	11.263
35,000	11.841	11.827	11.824	11.823	11.823
40,000	12.586	12.435	12.403	12.396	12.394
45,000	14.254	13.225	13.036	12.998	12.987
50,000	19.250	14.728	13.838	13.655	13.616

**Table B.16** Internal partition function of  $O^{+3}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	3.027	3.027	3.027	3.027	3.027
200	3.436	3.436	3.436	3.436	3.436
300	4.100	4.100	4.100	4.100	4.100
400	4.747	4.747	4.747	4.747	4.747
500	5.306	5.306	5.306	5.306	5.306
600	5.775	5.775	5.775	5.775	5.775
700	6.167	6.167	6.167	6.167	6.167
800	6.497	6.497	6.497	6.497	6.497
900	6.777	6.777	6.777	6.777	6.777
1000	7.018	7.018	7.018	7.018	7.018
1500	7.834	7.834	7.834	7.834	7.834
2000	8.303	8.303	8.303	8.303	8.303
2500	8.606	8.606	8.606	8.606	8.606
3000	8.817	8.817	8.817	8.817	8.817
3500	8.973	8.973	8.973	8.973	8.973
4000	9.093	9.093	9.093	9.093	9.093
4500	9.187	9.187	9.187	9.187	9.187
5000	9.264	9.264	9.264	9.264	9.264
6000	9.381	9.381	9.381	9.381	9.381
7000	9.466	9.466	9.466	9.466	9.466
8000	9.531	9.531	9.531	9.531	9.531
9000	9.581	9.581	9.581	9.581	9.581
10000	9.623	9.623	9.623	9.623	9.623
11000	9.657	9.657	9.657	9.657	9.657
12000	9.687	9.687	9.687	9.687	9.687
13000	9.715	9.715	9.715	9.715	9.715
14000	9.741	9.741	9.741	9.741	9.741
15000	9.767	9.767	9.767	9.767	9.767
16000	9.795	9.795	9.795	9.795	9.795
17000	9.824	9.824	9.824	9.824	9.824
18000	9.856	9.856	9.856	9.856	9.856
19000	9.892	9.892	9.892	9.892	9.892
20000	9.932	9.932	9.932	9.932	9.932
22000	10.024	10.024	10.024	10.024	10.024
24000	10.136	10.136	10.136	10.136	10.136
26000	10.267	10.267	10.267	10.267	10.267
28000	10.419	10.419	10.419	10.419	10.419
30000	10.592	10.592	10.592	10.592	10.592
35000	11.102	11.102	11.102	11.102	11.102
40000	11.714	11.714	11.714	11.714	11.714
45000	12.408	12.407	12.407	12.407	12.407
50000	13.174	13.168	13.167	13.166	13.166

**Table B.17** Internal partition function of  $O^{+4}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.000	1.000	1.000	1.000	1.000
200	1.000	1.000	1.000	1.000	1.000
300	1.000	1.000	1.000	1.000	1.000
400	1.000	1.000	1.000	1.000	1.000
500	1.000	1.000	1.000	1.000	1.000
600	1.000	1.000	1.000	1.000	1.000
700	1.000	1.000	1.000	1.000	1.000
800	1.000	1.000	1.000	1.000	1.000
900	1.000	1.000	1.000	1.000	1.000
1,000	1.000	1.000	1.000	1.000	1.000
1,500	1.000	1.000	1.000	1.000	1.000
2,000	1.000	1.000	1.000	1.000	1.000
2,500	1.000	1.000	1.000	1.000	1.000
3,000	1.000	1.000	1.000	1.000	1.000
3,500	1.000	1.000	1.000	1.000	1.000
4,000	1.000	1.000	1.000	1.000	1.000
4,500	1.000	1.000	1.000	1.000	1.000
5,000	1.000	1.000	1.000	1.000	1.000
6,000	1.000	1.000	1.000	1.000	1.000
7,000	1.000	1.000	1.000	1.000	1.000
8,000	1.000	1.000	1.000	1.000	1.000
9,000	1.000	1.000	1.000	1.000	1.000
10,000	1.000	1.000	1.000	1.000	1.000
11,000	1.000	1.000	1.000	1.000	1.000
12,000	1.000	1.000	1.000	1.000	1.000
13,000	1.001	1.001	1.001	1.001	1.001
14,000	1.002	1.002	1.002	1.002	1.002
15,000	1.003	1.003	1.003	1.003	1.003
16,000	1.006	1.006	1.006	1.006	1.006
17,000	1.009	1.009	1.009	1.009	1.009
18,000	1.013	1.013	1.013	1.013	1.013
19,000	1.018	1.018	1.018	1.018	1.018
20,000	1.024	1.024	1.024	1.024	1.024
22,000	1.042	1.042	1.042	1.042	1.042
24,000	1.065	1.065	1.065	1.065	1.065
26,000	1.096	1.096	1.096	1.096	1.096
28,000	1.133	1.133	1.133	1.133	1.133
30,000	1.176	1.176	1.176	1.176	1.176
35,000	1.312	1.312	1.312	1.312	1.312
40,000	1.483	1.483	1.483	1.483	1.483
45,000	1.681	1.681	1.681	1.681	1.681
50,000	1.901	1.901	1.901	1.901	1.901

### B.3 Selfconsistent Partition Functions of Atomic Species in Mars Atmosphere

**Table B.18** Internal partition function of  $C$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	6.047	6.047	6.047	6.047	6.047
200	7.325	7.325	7.325	7.325	7.325
300	7.834	7.834	7.834	7.834	7.834
400	8.105	8.105	8.105	8.105	8.105
500	8.275	8.275	8.275	8.275	8.275
600	8.390	8.390	8.390	8.390	8.390
700	8.474	8.474	8.474	8.474	8.474
800	8.537	8.537	8.537	8.537	8.537
900	8.587	8.587	8.587	8.587	8.587
1000	8.627	8.627	8.627	8.627	8.627
1500	8.750	8.750	8.750	8.750	8.750
2000	8.814	8.814	8.814	8.814	8.814
2500	8.863	8.863	8.863	8.863	8.863
3000	8.911	8.911	8.911	8.911	8.911
3500	8.967	8.967	8.967	8.967	8.967
4000	9.033	9.033	9.033	9.033	9.033
4500	9.109	9.109	9.109	9.109	9.109
5000	9.192	9.192	9.192	9.192	9.192
6000	9.378	9.378	9.378	9.378	9.378
7000	9.578	9.578	9.578	9.578	9.578
8000	9.794	9.787	9.785	9.785	9.785
9000	10.059	10.015	10.001	9.996	9.995
10000	10.506	10.296	10.235	10.215	10.209
11000	11.314	10.645	10.499	10.450	10.429
12000	13.039	11.233	10.808	10.699	10.664
13000	16.402	12.046	11.188	10.994	10.903
14000	23.527	13.513	11.726	11.291	11.170
15000	36.631	16.531	12.505	11.693	11.473
16000	59.096	20.524	13.591	12.197	11.751
17000	95.356	28.253	15.071	12.820	12.066
18000	150.983	37.545	17.064	13.361	12.462
19000	215.735	55.117	19.811	14.209	12.907
20000	323.235	72.823	25.318	15.448	13.411
22000	575.124	137.332	36.182	18.752	14.584
24000	934.721	216.856	59.810	22.829	16.026
26000	1527.220	322.346	84.249	28.147	17.778
28000	2351.650	455.038	114.686	35.746	19.775
30000	3450.040	697.270	151.049	45.106	22.015
35000	6892.110	1449.310	267.842	82.834	30.906
40000	11781.900	2297.410	504.874	122.770	43.203
45000	19413.000	3703.310	717.414	168.181	54.469
50000	27720.300	5535.600	986.138	222.399	75.323



**Table B.19** Internal partition function of  $C^+$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	3.606	3.606	3.606	3.606	3.606
200	4.535	4.535	4.535	4.535	4.535
300	4.951	4.951	4.951	4.951	4.951
400	5.184	5.184	5.184	5.184	5.184
500	5.333	5.333	5.333	5.333	5.333
600	5.436	5.436	5.436	5.436	5.436
700	5.511	5.511	5.511	5.511	5.511
800	5.569	5.569	5.569	5.569	5.569
900	5.614	5.614	5.614	5.614	5.614
1,000	5.651	5.651	5.651	5.651	5.651
1,500	5.764	5.764	5.764	5.764	5.764
2,000	5.822	5.822	5.822	5.822	5.822
2,500	5.857	5.857	5.857	5.857	5.857
3,000	5.880	5.880	5.880	5.880	5.880
3,500	5.897	5.897	5.897	5.897	5.897
4,000	5.910	5.910	5.910	5.910	5.910
4,500	5.920	5.920	5.920	5.920	5.920
5,000	5.928	5.928	5.928	5.928	5.928
6,000	5.940	5.940	5.940	5.940	5.940
7,000	5.950	5.950	5.950	5.950	5.950
8,000	5.960	5.960	5.960	5.960	5.960
9,000	5.972	5.972	5.972	5.972	5.972
10,000	5.988	5.988	5.988	5.988	5.988
11,000	6.011	6.011	6.011	6.011	6.011
12,000	6.040	6.040	6.040	6.040	6.040
13,000	6.077	6.077	6.077	6.077	6.077
14,000	6.123	6.123	6.123	6.123	6.123
15,000	6.178	6.177	6.177	6.177	6.177
16,000	6.242	6.241	6.240	6.240	6.240
17,000	6.317	6.313	6.312	6.312	6.312
18,000	6.406	6.395	6.393	6.392	6.392
19,000	6.514	6.487	6.482	6.481	6.480
20,000	6.648	6.591	6.579	6.577	6.576
22,000	7.063	6.849	6.803	6.793	6.791
24,000	7.826	7.201	7.070	7.040	7.033
26,000	9.372	7.715	7.405	7.324	7.302
28,000	12.341	8.578	7.819	7.643	7.598
30,000	18.241	9.835	8.350	8.008	7.921
35,000	52.700	17.567	10.477	9.174	8.891
40,000	136.351	35.910	15.086	10.864	10.084
45,000	316.524	72.906	24.128	13.760	11.554
50,000	641.095	137.719	36.760	17.431	13.382

**Table B.20** Internal partition function of  $C^{+2}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.000	1.000	1.000	1.000	1.000
200	1.000	1.000	1.000	1.000	1.000
300	1.000	1.000	1.000	1.000	1.000
400	1.000	1.000	1.000	1.000	1.000
500	1.000	1.000	1.000	1.000	1.000
600	1.000	1.000	1.000	1.000	1.000
700	1.000	1.000	1.000	1.000	1.000
800	1.000	1.000	1.000	1.000	1.000
900	1.000	1.000	1.000	1.000	1.000
1000	1.000	1.000	1.000	1.000	1.000
1500	1.000	1.000	1.000	1.000	1.000
2000	1.000	1.000	1.000	1.000	1.000
2500	1.000	1.000	1.000	1.000	1.000
3000	1.000	1.000	1.000	1.000	1.000
3500	1.000	1.000	1.000	1.000	1.000
4000	1.000	1.000	1.000	1.000	1.000
4500	1.000	1.000	1.000	1.000	1.000
5000	1.000	1.000	1.000	1.000	1.000
6000	1.000	1.000	1.000	1.000	1.000
7000	1.000	1.000	1.000	1.000	1.000
8000	1.001	1.001	1.001	1.001	1.001
9000	1.002	1.002	1.002	1.002	1.002
10000	1.005	1.005	1.005	1.005	1.005
11000	1.009	1.009	1.009	1.009	1.009
12000	1.017	1.017	1.017	1.017	1.017
13000	1.027	1.027	1.027	1.027	1.027
14000	1.041	1.041	1.041	1.041	1.041
15000	1.059	1.059	1.059	1.059	1.059
16000	1.081	1.081	1.081	1.081	1.081
17000	1.107	1.107	1.107	1.107	1.107
18000	1.137	1.137	1.137	1.137	1.137
19000	1.172	1.172	1.172	1.172	1.172
20000	1.210	1.210	1.210	1.210	1.210
22000	1.297	1.297	1.297	1.297	1.297
24000	1.398	1.398	1.398	1.398	1.398
26000	1.512	1.511	1.511	1.511	1.511
28000	1.636	1.635	1.635	1.635	1.635
30000	1.772	1.769	1.768	1.768	1.768
35000	2.200	2.147	2.137	2.134	2.134
40000	3.037	2.645	2.561	2.543	2.539
45000	5.601	3.505	3.081	3.001	2.979
50000	13.175	5.381	3.847	3.532	3.463

**Table B.21** Internal partition function of  $C^{+3}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.000	2.000	2.000	2.000	2.000
200	2.000	2.000	2.000	2.000	2.000
300	2.000	2.000	2.000	2.000	2.000
400	2.000	2.000	2.000	2.000	2.000
500	2.000	2.000	2.000	2.000	2.000
600	2.000	2.000	2.000	2.000	2.000
700	2.000	2.000	2.000	2.000	2.000
800	2.000	2.000	2.000	2.000	2.000
900	2.000	2.000	2.000	2.000	2.000
1,000	2.000	2.000	2.000	2.000	2.000
1,500	2.000	2.000	2.000	2.000	2.000
2,000	2.000	2.000	2.000	2.000	2.000
2,500	2.000	2.000	2.000	2.000	2.000
3,000	2.000	2.000	2.000	2.000	2.000
3,500	2.000	2.000	2.000	2.000	2.000
4,000	2.000	2.000	2.000	2.000	2.000
4,500	2.000	2.000	2.000	2.000	2.000
5,000	2.000	2.000	2.000	2.000	2.000
6,000	2.000	2.000	2.000	2.000	2.000
7,000	2.000	2.000	2.000	2.000	2.000
8,000	2.000	2.000	2.000	2.000	2.000
9,000	2.000	2.000	2.000	2.000	2.000
10,000	2.001	2.001	2.001	2.001	2.001
11,000	2.001	2.001	2.001	2.001	2.001
12,000	2.003	2.003	2.003	2.003	2.003
13,000	2.005	2.005	2.005	2.005	2.005
14,000	2.008	2.008	2.008	2.008	2.008
15,000	2.012	2.012	2.012	2.012	2.012
16,000	2.018	2.018	2.018	2.018	2.018
17,000	2.025	2.025	2.025	2.025	2.025
18,000	2.034	2.034	2.034	2.034	2.034
19,000	2.045	2.045	2.045	2.045	2.045
20,000	2.058	2.058	2.058	2.058	2.058
22,000	2.088	2.088	2.088	2.088	2.088
24,000	2.125	2.125	2.125	2.125	2.125
26,000	2.169	2.169	2.169	2.169	2.169
28,000	2.218	2.218	2.218	2.218	2.218
30,000	2.271	2.271	2.271	2.271	2.271
35,000	2.423	2.422	2.422	2.422	2.422
40,000	2.592	2.589	2.589	2.589	2.589
45,000	2.791	2.768	2.764	2.763	2.763
50,000	3.097	2.971	2.945	2.940	2.939

**Table B.22** Internal partition function of  $N$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	4.000	4.000	4.000	4.000	4.000
200	4.000	4.000	4.000	4.000	4.000
300	4.000	4.000	4.000	4.000	4.000
400	4.000	4.000	4.000	4.000	4.000
500	4.000	4.000	4.000	4.000	4.000
600	4.000	4.000	4.000	4.000	4.000
700	4.000	4.000	4.000	4.000	4.000
800	4.000	4.000	4.000	4.000	4.000
900	4.000	4.000	4.000	4.000	4.000
1000	4.000	4.000	4.000	4.000	4.000
1500	4.000	4.000	4.000	4.000	4.000
2000	4.000	4.000	4.000	4.000	4.000
2500	4.000	4.000	4.000	4.000	4.000
3000	4.001	4.001	4.001	4.001	4.001
3500	4.004	4.004	4.004	4.004	4.004
4000	4.010	4.010	4.010	4.010	4.010
4500	4.022	4.022	4.022	4.022	4.022
5000	4.041	4.041	4.041	4.041	4.041
6000	4.105	4.105	4.105	4.105	4.105
7000	4.208	4.208	4.208	4.208	4.208
8000	4.349	4.348	4.348	4.348	4.348
9000	4.524	4.523	4.522	4.522	4.522
10000	4.734	4.727	4.725	4.724	4.724
11000	4.990	4.958	4.951	4.949	4.948
12000	5.339	5.226	5.199	5.192	5.190
13000	5.886	5.538	5.470	5.453	5.446
14000	6.933	5.946	5.770	5.726	5.715
15000	8.969	6.593	6.117	6.021	5.996
16000	13.421	7.496	6.535	6.342	6.279
17000	19.851	9.189	7.055	6.697	6.576
18000	31.899	11.416	7.720	7.075	6.891
19000	48.156	15.737	8.684	7.522	7.224
20000	76.701	20.827	10.246	8.098	7.579
22000	157.071	40.912	14.091	9.476	8.366
24000	290.849	70.806	21.609	11.361	9.290
26000	533.113	115.802	33.418	13.991	10.400
28000	908.347	178.946	48.161	17.828	11.690
30000	1456.560	262.752	67.473	23.687	13.217
35000	3482.800	734.684	138.765	45.545	18.921
40000	6818.060	1330.920	295.223	73.924	28.148
45000	12485.900	2382.080	464.643	111.993	42.185
50000	19402.700	3873.690	713.616	157.473	56.313

**Table B.23** Internal partition function of  $N^+$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	3.250	3.250	3.250	3.250	3.250
200	5.065	5.065	5.065	5.065	5.065
300	6.045	6.045	6.045	6.045	6.045
400	6.641	6.641	6.641	6.641	6.641
500	7.039	7.039	7.039	7.039	7.039
600	7.323	7.323	7.323	7.323	7.323
700	7.536	7.536	7.536	7.536	7.536
800	7.700	7.700	7.700	7.700	7.700
900	7.832	7.832	7.832	7.832	7.832
1,000	7.939	7.939	7.939	7.939	7.939
1,500	8.274	8.274	8.274	8.274	8.274
2,000	8.448	8.448	8.448	8.448	8.448
2,500	8.555	8.555	8.555	8.555	8.555
3,000	8.630	8.630	8.630	8.630	8.630
3,500	8.688	8.688	8.688	8.688	8.688
4,000	8.738	8.738	8.738	8.738	8.738
4,500	8.786	8.786	8.786	8.786	8.786
5,000	8.835	8.835	8.835	8.835	8.835
6,000	8.938	8.938	8.938	8.938	8.938
7,000	9.054	9.054	9.054	9.054	9.054
8,000	9.180	9.180	9.180	9.180	9.180
9,000	9.314	9.314	9.314	9.314	9.314
10,000	9.453	9.453	9.453	9.453	9.453
11,000	9.596	9.596	9.596	9.596	9.596
12,000	9.740	9.740	9.740	9.740	9.740
13,000	9.886	9.886	9.886	9.886	9.886
14,000	10.031	10.031	10.031	10.031	10.031
15,000	10.177	10.177	10.177	10.177	10.177
16,000	10.322	10.321	10.321	10.321	10.321
17,000	10.467	10.466	10.466	10.466	10.466
18,000	10.613	10.610	10.610	10.610	10.610
19,000	10.763	10.755	10.753	10.753	10.753
20,000	10.920	10.901	10.897	10.896	10.896
22,000	11.304	11.207	11.187	11.183	11.182
24,000	11.941	11.559	11.489	11.475	11.472
26,000	13.249	12.029	11.826	11.778	11.766
28,000	16.278	12.742	12.222	12.102	12.071
30,000	22.390	14.048	12.731	12.459	12.391
35,000	72.363	23.333	15.019	13.638	13.342
40,000	225.137	51.463	21.169	15.734	14.601
45,000	640.863	119.811	35.915	19.772	16.369
50,000	1,478.330	258.378	60.511	26.071	18.844

**Table B.24** Internal partition function of  $N^{+2}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.325	2.325	2.325	2.325	2.325
200	3.141	3.141	3.141	3.141	3.141
300	3.733	3.733	3.733	3.733	3.733
400	4.136	4.136	4.136	4.136	4.136
500	4.422	4.422	4.422	4.422	4.422
600	4.633	4.633	4.633	4.633	4.633
700	4.795	4.795	4.795	4.795	4.795
800	4.923	4.923	4.923	4.923	4.923
900	5.027	5.027	5.027	5.027	5.027
1000	5.112	5.112	5.112	5.112	5.112
1500	5.384	5.384	5.384	5.384	5.384
2000	5.528	5.528	5.528	5.528	5.528
2500	5.618	5.618	5.618	5.618	5.618
3000	5.679	5.679	5.679	5.679	5.679
3500	5.723	5.723	5.723	5.723	5.723
4000	5.757	5.757	5.757	5.757	5.757
4500	5.783	5.783	5.783	5.783	5.783
5000	5.804	5.804	5.804	5.804	5.804
6000	5.836	5.836	5.836	5.836	5.836
7000	5.859	5.859	5.859	5.859	5.859
8000	5.877	5.877	5.877	5.877	5.877
9000	5.891	5.891	5.891	5.891	5.891
10000	5.904	5.904	5.904	5.904	5.904
11000	5.917	5.917	5.917	5.917	5.917
12000	5.930	5.930	5.930	5.930	5.930
13000	5.945	5.945	5.945	5.945	5.945
14000	5.963	5.963	5.963	5.963	5.963
15000	5.984	5.984	5.984	5.984	5.984
16000	6.008	6.008	6.008	6.008	6.008
17000	6.038	6.038	6.038	6.038	6.038
18000	6.071	6.071	6.071	6.071	6.071
19000	6.109	6.109	6.109	6.109	6.109
20000	6.152	6.152	6.152	6.152	6.152
22000	6.252	6.252	6.252	6.252	6.252
24000	6.371	6.371	6.371	6.371	6.371
26000	6.507	6.507	6.507	6.507	6.507
28000	6.660	6.659	6.659	6.659	6.659
30000	6.831	6.826	6.826	6.825	6.825
35000	7.382	7.308	7.299	7.298	7.298
40000	8.494	7.909	7.849	7.838	7.836
45000	12.053	8.787	8.494	8.442	8.429
50000	23.634	10.443	9.315	9.115	9.076

**Table B.25** Internal partition function of  $N^{+3}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.000	1.000	1.000	1.000	1.000
200	1.000	1.000	1.000	1.000	1.000
300	1.000	1.000	1.000	1.000	1.000
400	1.000	1.000	1.000	1.000	1.000
500	1.000	1.000	1.000	1.000	1.000
600	1.000	1.000	1.000	1.000	1.000
700	1.000	1.000	1.000	1.000	1.000
800	1.000	1.000	1.000	1.000	1.000
900	1.000	1.000	1.000	1.000	1.000
1,000	1.000	1.000	1.000	1.000	1.000
1,500	1.000	1.000	1.000	1.000	1.000
2,000	1.000	1.000	1.000	1.000	1.000
2,500	1.000	1.000	1.000	1.000	1.000
3,000	1.000	1.000	1.000	1.000	1.000
3,500	1.000	1.000	1.000	1.000	1.000
4,000	1.000	1.000	1.000	1.000	1.000
4,500	1.000	1.000	1.000	1.000	1.000
5,000	1.000	1.000	1.000	1.000	1.000
6,000	1.000	1.000	1.000	1.000	1.000
7,000	1.000	1.000	1.000	1.000	1.000
8,000	1.000	1.000	1.000	1.000	1.000
9,000	1.000	1.000	1.000	1.000	1.000
10,000	1.001	1.001	1.001	1.001	1.001
11,000	1.001	1.001	1.001	1.001	1.001
12,000	1.003	1.003	1.003	1.003	1.003
13,000	1.005	1.005	1.005	1.005	1.005
14,000	1.009	1.009	1.009	1.009	1.009
15,000	1.014	1.014	1.014	1.014	1.014
16,000	1.021	1.021	1.021	1.021	1.021
17,000	1.030	1.030	1.030	1.030	1.030
18,000	1.041	1.041	1.041	1.041	1.041
19,000	1.055	1.055	1.055	1.055	1.055
20,000	1.071	1.071	1.071	1.071	1.071
22,000	1.111	1.111	1.111	1.111	1.111
24,000	1.160	1.160	1.160	1.160	1.160
26,000	1.219	1.219	1.219	1.219	1.219
28,000	1.287	1.287	1.287	1.287	1.287
30,000	1.364	1.364	1.364	1.364	1.364
35,000	1.585	1.585	1.585	1.585	1.585
40,000	1.842	1.842	1.842	1.842	1.842
45,000	2.127	2.126	2.125	2.125	2.125
50,000	2.443	2.431	2.428	2.428	2.428

**Table B.26** Internal partition function of  $N^{+4}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.000	2.000	2.000	2.000	2.000
200	2.000	2.000	2.000	2.000	2.000
300	2.000	2.000	2.000	2.000	2.000
400	2.000	2.000	2.000	2.000	2.000
500	2.000	2.000	2.000	2.000	2.000
600	2.000	2.000	2.000	2.000	2.000
700	2.000	2.000	2.000	2.000	2.000
800	2.000	2.000	2.000	2.000	2.000
900	2.000	2.000	2.000	2.000	2.000
1000	2.000	2.000	2.000	2.000	2.000
1500	2.000	2.000	2.000	2.000	2.000
2000	2.000	2.000	2.000	2.000	2.000
2500	2.000	2.000	2.000	2.000	2.000
3000	2.000	2.000	2.000	2.000	2.000
3500	2.000	2.000	2.000	2.000	2.000
4000	2.000	2.000	2.000	2.000	2.000
4500	2.000	2.000	2.000	2.000	2.000
5000	2.000	2.000	2.000	2.000	2.000
6000	2.000	2.000	2.000	2.000	2.000
7000	2.000	2.000	2.000	2.000	2.000
8000	2.000	2.000	2.000	2.000	2.000
9000	2.000	2.000	2.000	2.000	2.000
10000	2.000	2.000	2.000	2.000	2.000
11000	2.000	2.000	2.000	2.000	2.000
12000	2.000	2.000	2.000	2.000	2.000
13000	2.001	2.001	2.001	2.001	2.001
14000	2.002	2.002	2.002	2.002	2.002
15000	2.003	2.003	2.003	2.003	2.003
16000	2.004	2.004	2.004	2.004	2.004
17000	2.007	2.007	2.007	2.007	2.007
18000	2.010	2.010	2.010	2.010	2.010
19000	2.013	2.013	2.013	2.013	2.013
20000	2.018	2.018	2.018	2.018	2.018
22000	2.031	2.031	2.031	2.031	2.031
24000	2.048	2.048	2.048	2.048	2.048
26000	2.069	2.069	2.069	2.069	2.069
28000	2.095	2.095	2.095	2.095	2.095
30000	2.126	2.126	2.126	2.126	2.126
35000	2.218	2.218	2.218	2.218	2.218
40000	2.330	2.330	2.330	2.330	2.330
45000	2.456	2.456	2.456	2.456	2.456
50000	2.590	2.589	2.589	2.589	2.589



**Table B.27** Internal partition function of *O* as a function of pressure and temperature

<i>T</i> (K)	<i>P</i> (bar)				
	10 <sup>-2</sup>	10 <sup>-1</sup>	1	10 <sup>1</sup>	10 <sup>2</sup>
100	5.346	5.346	5.346	5.346	5.346
200	6.156	6.156	6.156	6.156	6.156
300	6.741	6.741	6.741	6.741	6.741
400	7.140	7.140	7.140	7.140	7.140
500	7.423	7.423	7.423	7.423	7.423
600	7.633	7.633	7.633	7.633	7.633
700	7.794	7.794	7.794	7.794	7.794
800	7.922	7.922	7.922	7.922	7.922
900	8.025	8.025	8.025	8.025	8.025
1,000	8.110	8.110	8.110	8.110	8.110
1,500	8.382	8.382	8.382	8.382	8.382
2,000	8.527	8.527	8.527	8.527	8.527
2,500	8.617	8.617	8.617	8.617	8.617
3,000	8.680	8.680	8.680	8.680	8.680
3,500	8.729	8.729	8.729	8.729	8.729
4,000	8.772	8.772	8.772	8.772	8.772
4,500	8.813	8.813	8.813	8.813	8.813
5,000	8.855	8.855	8.855	8.855	8.855
6,000	8.947	8.947	8.947	8.947	8.947
7,000	9.051	9.051	9.051	9.051	9.051
8,000	9.166	9.166	9.166	9.166	9.166
9,000	9.292	9.290	9.290	9.290	9.290
10,000	9.432	9.422	9.422	9.420	9.418
11,000	9.601	9.565	9.565	9.555	9.550
12,000	9.850	9.733	9.732	9.694	9.685
13,000	10.275	9.952	9.950	9.837	9.819
14,000	11.144	10.271	10.266	9.985	9.956
15,000	12.845	10.761	10.750	10.141	10.098
16,000	16.020	11.518	11.497	10.323	10.233
17,000	21.614	12.669	12.628	10.539	10.375
18,000	30.941	14.352	14.285	10.800	10.528
19,000	43.050	17.610	16.637	11.118	10.692
20,000	63.931	21.312	19.839	11.508	10.868
22,000	119.886	35.529	29.536	12.578	11.268
24,000	209.062	55.669	44.835	14.986	11.748
26,000	365.905	84.897	66.939	17.715	12.323
28,000	601.422	124.622	96.927	24.212	13.003
30,000	936.450	175.889	135.577	30.131	13.795
35,000	2,118.650	455.643	272.798	50.405	16.906
40,000	3,983.830	788.986	468.622	97.460	23.395
45,000	6,609.160	1,363.260	716.958	169.424	29.194
50,000	10,723.700	2,157.420	1,011.150	239.463	38.069

**Table B.28** Internal partition function of  $O^+$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	4.000	4.000	4.000	4.000	4.000
200	4.000	4.000	4.000	4.000	4.000
300	4.000	4.000	4.000	4.000	4.000
400	4.000	4.000	4.000	4.000	4.000
500	4.000	4.000	4.000	4.000	4.000
600	4.000	4.000	4.000	4.000	4.000
700	4.000	4.000	4.000	4.000	4.000
800	4.000	4.000	4.000	4.000	4.000
900	4.000	4.000	4.000	4.000	4.000
1000	4.000	4.000	4.000	4.000	4.000
1500	4.000	4.000	4.000	4.000	4.000
2000	4.000	4.000	4.000	4.000	4.000
2500	4.000	4.000	4.000	4.000	4.000
3000	4.000	4.000	4.000	4.000	4.000
3500	4.000	4.000	4.000	4.000	4.000
4000	4.001	4.001	4.001	4.001	4.001
4500	4.002	4.002	4.002	4.002	4.002
5000	4.005	4.005	4.005	4.005	4.005
6000	4.016	4.016	4.016	4.016	4.016
7000	4.042	4.042	4.042	4.042	4.042
8000	4.085	4.085	4.085	4.085	4.085
9000	4.147	4.147	4.147	4.147	4.147
10000	4.229	4.229	4.229	4.229	4.229
11000	4.330	4.330	4.330	4.330	4.330
12000	4.448	4.448	4.448	4.448	4.448
13000	4.582	4.582	4.582	4.582	4.582
14000	4.729	4.729	4.729	4.729	4.729
15000	4.887	4.887	4.887	4.887	4.887
16000	5.055	5.055	5.055	5.055	5.055
17000	5.230	5.229	5.229	5.229	5.229
18000	5.412	5.409	5.409	5.409	5.409
19000	5.607	5.594	5.594	5.594	5.594
20000	5.833	5.781	5.781	5.781	5.781
22000	6.594	6.163	6.162	6.162	6.162
24000	8.569	6.552	6.546	6.546	6.544
26000	14.406	6.953	6.931	6.931	6.926
28000	30.234	7.395	7.321	7.320	7.304
30000	68.213	7.920	7.723	7.721	7.680
35000	430.487	10.831	8.913	8.899	8.627
40000	1819.130	20.863	10.842	10.794	9.648
45000	5626.660	48.597	14.500	14.407	10.868
50000	13908.700	130.543	21.288	21.099	12.468

**Table B.29** Internal partition function of  $O^{+2}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.650	1.650	1.650	1.650	1.650
200	2.882	2.882	2.882	2.882	2.882
300	3.895	3.895	3.895	3.895	3.895
400	4.659	4.659	4.659	4.659	4.659
500	5.238	5.238	5.238	5.238	5.238
600	5.686	5.686	5.686	5.686	5.686
700	6.042	6.042	6.042	6.042	6.042
800	6.330	6.330	6.330	6.330	6.330
900	6.568	6.568	6.568	6.568	6.568
1,000	6.768	6.768	6.768	6.768	6.768
1,500	7.419	7.419	7.419	7.419	7.419
2,000	7.777	7.777	7.777	7.777	7.777
2,500	8.003	8.003	8.003	8.003	8.003
3,000	8.159	8.159	8.159	8.159	8.159
3,500	8.274	8.274	8.274	8.274	8.274
4,000	8.362	8.362	8.362	8.362	8.362
4,500	8.435	8.435	8.435	8.435	8.435
5,000	8.497	8.497	8.497	8.497	8.497
6,000	8.604	8.604	8.604	8.604	8.604
7,000	8.704	8.704	8.704	8.704	8.704
8,000	8.803	8.803	8.803	8.803	8.803
9,000	8.904	8.904	8.904	8.904	8.904
10,000	9.009	9.009	9.009	9.009	9.009
11,000	9.118	9.118	9.118	9.118	9.118
12,000	9.228	9.228	9.228	9.228	9.228
13,000	9.341	9.341	9.341	9.341	9.341
14,000	9.455	9.455	9.455	9.455	9.455
15,000	9.570	9.570	9.570	9.570	9.570
16,000	9.684	9.684	9.684	9.684	9.684
17,000	9.799	9.799	9.799	9.799	9.799
18,000	9.914	9.914	9.914	9.914	9.914
19,000	10.029	10.029	10.029	10.029	10.029
20,000	10.143	10.143	10.143	10.143	10.143
22,000	10.369	10.369	10.369	10.369	10.369
24,000	10.594	10.594	10.594	10.594	10.594
26,000	10.818	10.818	10.818	10.818	10.818
28,000	11.041	11.041	11.041	11.041	11.041
30,000	11.263	11.263	11.263	11.263	11.263
35,000	11.824	11.823	11.823	11.823	11.822
40,000	12.410	12.401	12.399	12.398	12.393
45,000	13.078	13.026	13.014	13.013	12.984
50,000	13.988	13.795	13.724	13.720	13.602

**Table B.30** Internal partition function of  $O^{+3}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.016	2.016	2.016	2.016	2.016
200	2.249	2.249	2.249	2.249	2.249
300	2.628	2.628	2.628	2.628	2.628
400	2.998	2.998	2.998	2.998	2.998
500	3.318	3.318	3.318	3.318	3.318
600	3.586	3.586	3.586	3.586	3.586
700	3.810	3.810	3.810	3.810	3.810
800	3.998	3.998	3.998	3.998	3.998
900	4.158	4.158	4.158	4.158	4.158
1000	4.296	4.296	4.296	4.296	4.296
1500	4.763	4.763	4.763	4.763	4.763
2000	5.030	5.030	5.030	5.030	5.030
2500	5.203	5.203	5.203	5.203	5.203
3000	5.324	5.324	5.324	5.324	5.324
3500	5.413	5.413	5.413	5.413	5.413
4000	5.482	5.482	5.482	5.482	5.482
4500	5.536	5.536	5.536	5.536	5.536
5000	5.580	5.580	5.580	5.580	5.580
6000	5.646	5.646	5.646	5.646	5.646
7000	5.695	5.695	5.695	5.695	5.695
8000	5.732	5.732	5.732	5.732	5.732
9000	5.761	5.761	5.761	5.761	5.761
10000	5.784	5.784	5.784	5.784	5.784
11000	5.804	5.804	5.804	5.804	5.804
12000	5.821	5.821	5.821	5.821	5.821
13000	5.837	5.837	5.837	5.837	5.837
14000	5.852	5.852	5.852	5.852	5.852
15000	5.867	5.867	5.867	5.867	5.867
16000	5.883	5.883	5.883	5.883	5.883
17000	5.900	5.900	5.900	5.900	5.900
18000	5.918	5.918	5.918	5.918	5.918
19000	5.938	5.938	5.938	5.938	5.938
20000	5.961	5.961	5.961	5.961	5.961
22000	6.014	6.014	6.014	6.014	6.014
24000	6.077	6.077	6.077	6.077	6.077
26000	6.153	6.153	6.153	6.153	6.153
28000	6.239	6.239	6.239	6.239	6.239
30000	6.338	6.338	6.338	6.338	6.338
35000	6.629	6.629	6.629	6.629	6.629
40000	6.978	6.978	6.978	6.978	6.978
45000	7.373	7.373	7.373	7.373	7.373
50000	7.808	7.807	7.807	7.807	7.806

**Table B.31** Internal partition function of  $O^{+4}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.000	1.000	1.000	1.000	1.000
200	1.000	1.000	1.000	1.000	1.000
300	1.000	1.000	1.000	1.000	1.000
400	1.000	1.000	1.000	1.000	1.000
500	1.000	1.000	1.000	1.000	1.000
600	1.000	1.000	1.000	1.000	1.000
700	1.000	1.000	1.000	1.000	1.000
800	1.000	1.000	1.000	1.000	1.000
900	1.000	1.000	1.000	1.000	1.000
1000	1.000	1.000	1.000	1.000	1.000
1,500	1.000	1.000	1.000	1.000	1.000
2,000	1.000	1.000	1.000	1.000	1.000
2,500	1.000	1.000	1.000	1.000	1.000
3,000	1.000	1.000	1.000	1.000	1.000
3,500	1.000	1.000	1.000	1.000	1.000
4,000	1.000	1.000	1.000	1.000	1.000
4,500	1.000	1.000	1.000	1.000	1.000
5,000	1.000	1.000	1.000	1.000	1.000
6,000	1.000	1.000	1.000	1.000	1.000
7,000	1.000	1.000	1.000	1.000	1.000
8,000	1.000	1.000	1.000	1.000	1.000
9,000	1.000	1.000	1.000	1.000	1.000
10,000	1.000	1.000	1.000	1.000	1.000
11,000	1.000	1.000	1.000	1.000	1.000
12,000	1.000	1.000	1.000	1.000	1.000
13,000	1.001	1.001	1.001	1.001	1.001
14,000	1.002	1.002	1.002	1.002	1.002
15,000	1.003	1.003	1.003	1.003	1.003
16,000	1.006	1.006	1.006	1.006	1.006
17,000	1.009	1.009	1.009	1.009	1.009
18,000	1.013	1.013	1.013	1.013	1.013
19,000	1.018	1.018	1.018	1.018	1.018
20,000	1.024	1.024	1.024	1.024	1.024
22,000	1.042	1.042	1.042	1.042	1.042
24,000	1.065	1.065	1.065	1.065	1.065
26,000	1.096	1.096	1.096	1.096	1.096
28,000	1.133	1.133	1.133	1.133	1.133
30,000	1.176	1.176	1.176	1.176	1.176
35,000	1.312	1.312	1.312	1.312	1.312
40,000	1.483	1.483	1.483	1.483	1.483
45,000	1.681	1.681	1.681	1.681	1.681
50,000	1.901	1.901	1.901	1.901	1.901

**Table B.32** Internal partition function of *Ar* as a function of pressure and temperature

<i>T</i> (K)	<i>P</i> (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.000	1.000	1.000	1.000	1.000
200	1.000	1.000	1.000	1.000	1.000
300	1.000	1.000	1.000	1.000	1.000
400	1.000	1.000	1.000	1.000	1.000
500	1.000	1.000	1.000	1.000	1.000
600	1.000	1.000	1.000	1.000	1.000
700	1.000	1.000	1.000	1.000	1.000
800	1.000	1.000	1.000	1.000	1.000
900	1.000	1.000	1.000	1.000	1.000
1000	1.000	1.000	1.000	1.000	1.000
1500	1.000	1.000	1.000	1.000	1.000
2000	1.000	1.000	1.000	1.000	1.000
2500	1.000	1.000	1.000	1.000	1.000
3000	1.000	1.000	1.000	1.000	1.000
3500	1.000	1.000	1.000	1.000	1.000
4000	1.000	1.000	1.000	1.000	1.000
4500	1.000	1.000	1.000	1.000	1.000
5000	1.000	1.000	1.000	1.000	1.000
6000	1.000	1.000	1.000	1.000	1.000
7000	1.000	1.000	1.000	1.000	1.000
8000	1.000	1.000	1.000	1.000	1.000
9000	1.000	1.000	1.000	1.000	1.000
10000	1.000	1.000	1.000	1.000	1.000
11000	1.002	1.002	1.001	1.000	1.000
12000	1.007	1.006	1.002	1.001	1.001
13000	1.021	1.016	1.006	1.003	1.002
14000	1.056	1.043	1.014	1.006	1.004
15000	1.133	1.115	1.031	1.013	1.008
16000	1.284	1.245	1.065	1.027	1.013
17000	1.551	1.545	1.126	1.049	1.023
18000	1.997	1.987	1.225	1.085	1.038
19000	2.694	2.681	1.456	1.140	1.059
20000	3.728	3.708	1.732	1.220	1.090
22000	7.220	7.175	2.659	1.488	1.178
24000	13.363	13.274	4.916	1.949	1.329
26000	23.119	22.952	7.988	2.685	1.586
28000	37.426	37.144	12.448	4.226	1.940
30000	57.132	56.697	18.590	6.182	2.437
35000	134.284	133.268	42.582	13.574	4.334
40000	256.011	254.101	96.117	24.788	8.588
45000	423.601	420.154	158.724	40.332	13.110
50000	633.946	628.876	281.687	59.970	18.614

**Table B.33** Internal partition function of  $Ar^+$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	4.000	4.000	4.000	4.000	4.000
200	4.000	4.000	4.000	4.000	4.000
300	4.002	4.002	4.002	4.002	4.002
400	4.012	4.012	4.012	4.012	4.012
500	4.033	4.033	4.033	4.033	4.033
600	4.065	4.065	4.065	4.065	4.065
700	4.105	4.105	4.105	4.105	4.105
800	4.152	4.152	4.152	4.152	4.152
900	4.203	4.203	4.203	4.203	4.203
1,000	4.255	4.255	4.255	4.255	4.255
1,500	4.507	4.507	4.507	4.507	4.507
2,000	4.714	4.714	4.714	4.714	4.714
2,500	4.877	4.877	4.877	4.877	4.877
3,000	5.007	5.007	5.007	5.007	5.007
3,500	5.110	5.110	5.110	5.110	5.110
4,000	5.195	5.195	5.195	5.195	5.195
4,500	5.265	5.265	5.265	5.265	5.265
5,000	5.325	5.325	5.325	5.325	5.325
6,000	5.419	5.419	5.419	5.419	5.419
7,000	5.490	5.490	5.490	5.490	5.490
8,000	5.546	5.546	5.546	5.546	5.546
9,000	5.591	5.591	5.591	5.591	5.591
10,000	5.628	5.628	5.628	5.628	5.628
11,000	5.658	5.658	5.658	5.658	5.658
12,000	5.685	5.685	5.685	5.685	5.685
13,000	5.707	5.707	5.707	5.707	5.707
14,000	5.726	5.726	5.726	5.726	5.726
15,000	5.744	5.744	5.744	5.744	5.744
16,000	5.759	5.759	5.759	5.759	5.759
17,000	5.773	5.773	5.773	5.773	5.773
18,000	5.787	5.787	5.787	5.786	5.786
19,000	5.801	5.801	5.800	5.799	5.799
20,000	5.817	5.817	5.815	5.812	5.812
22,000	5.864	5.862	5.856	5.844	5.841
24,000	5.957	5.950	5.930	5.891	5.880
26,000	6.150	6.132	6.092	5.975	5.939
28,000	6.540	6.491	6.395	6.115	6.030
30,000	7.252	7.148	6.941	6.351	6.167
35,000	11.742	11.489	10.365	7.689	6.891
40,000	23.458	22.662	20.771	10.847	8.382
45,000	47.438	45.501	41.158	18.050	10.995
50,000	88.945	84.930	76.092	29.737	15.160

**Table B.34** Internal partition function of  $Ar^{+2}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	5.597	5.597	5.597	5.597	5.597
200	6.339	6.339	6.339	6.339	6.339
300	6.752	6.752	6.752	6.752	6.752
400	7.007	7.007	7.007	7.007	7.007
500	7.183	7.183	7.183	7.183	7.183
600	7.316	7.316	7.316	7.316	7.316
700	7.422	7.422	7.422	7.422	7.422
800	7.511	7.511	7.511	7.511	7.511
900	7.589	7.589	7.589	7.589	7.589
1000	7.657	7.657	7.657	7.657	7.657
1500	7.916	7.916	7.916	7.916	7.916
2000	8.091	8.091	8.091	8.091	8.091
2500	8.219	8.219	8.219	8.219	8.219
3000	8.320	8.320	8.320	8.320	8.320
3500	8.405	8.405	8.405	8.405	8.405
4000	8.482	8.482	8.482	8.482	8.482
4500	8.556	8.556	8.556	8.556	8.556
5000	8.630	8.630	8.630	8.630	8.630
6000	8.781	8.781	8.781	8.781	8.781
7000	8.938	8.938	8.938	8.938	8.938
8000	9.099	9.099	9.099	9.099	9.099
9000	9.262	9.262	9.262	9.262	9.262
10000	9.424	9.424	9.424	9.424	9.424
11000	9.584	9.584	9.584	9.584	9.584
12000	9.739	9.739	9.739	9.739	9.739
13000	9.889	9.889	9.889	9.889	9.889
14000	10.034	10.034	10.034	10.034	10.034
15000	10.174	10.174	10.174	10.174	10.174
16000	10.307	10.307	10.307	10.307	10.307
17000	10.435	10.435	10.435	10.435	10.435
18000	10.558	10.558	10.558	10.558	10.558
19000	10.676	10.676	10.676	10.676	10.676
20000	10.789	10.789	10.789	10.789	10.789
22000	11.004	11.004	11.004	11.004	11.004
24000	11.205	11.205	11.205	11.205	11.205
26000	11.398	11.398	11.398	11.397	11.397
28000	11.588	11.588	11.588	11.587	11.586
30000	11.781	11.781	11.781	11.779	11.777
35000	12.341	12.341	12.341	12.316	12.304
40000	13.181	13.181	13.181	13.058	12.988
45000	14.657	14.656	14.656	14.211	13.953
50000	17.318	17.317	17.317	16.198	15.341



**Table B.35** Internal partition function of  $Ar^{+3}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	4.000	4.000	4.000	4.000	4.000
200	4.000	4.000	4.000	4.000	4.000
300	4.000	4.000	4.000	4.000	4.000
400	4.000	4.000	4.000	4.000	4.000
500	4.000	4.000	4.000	4.000	4.000
600	4.000	4.000	4.000	4.000	4.000
700	4.000	4.000	4.000	4.000	4.000
800	4.000	4.000	4.000	4.000	4.000
900	4.000	4.000	4.000	4.000	4.000
1,000	4.000	4.000	4.000	4.000	4.000
1,500	4.000	4.000	4.000	4.000	4.000
2,000	4.000	4.000	4.000	4.000	4.000
2,500	4.000	4.000	4.000	4.000	4.000
3,000	4.000	4.000	4.000	4.000	4.000
3,500	4.002	4.002	4.002	4.002	4.002
4,000	4.005	4.005	4.005	4.005	4.005
4,500	4.012	4.012	4.012	4.012	4.012
5,000	4.023	4.023	4.023	4.023	4.023
6,000	4.064	4.064	4.064	4.064	4.064
7,000	4.134	4.134	4.134	4.134	4.134
8,000	4.233	4.233	4.233	4.233	4.233
9,000	4.362	4.362	4.362	4.362	4.362
10,000	4.515	4.515	4.515	4.515	4.515
11,000	4.689	4.689	4.689	4.689	4.689
12,000	4.881	4.881	4.881	4.881	4.881
13,000	5.086	5.086	5.086	5.086	5.086
14,000	5.301	5.301	5.301	5.301	5.301
15,000	5.523	5.523	5.523	5.523	5.523
16,000	5.749	5.749	5.749	5.749	5.749
17,000	5.979	5.979	5.979	5.979	5.979
18,000	6.209	6.209	6.209	6.209	6.209
19,000	6.440	6.440	6.440	6.440	6.440
20,000	6.669	6.669	6.669	6.669	6.669
22,000	7.121	7.121	7.121	7.121	7.121
24,000	7.561	7.561	7.561	7.561	7.561
26,000	7.989	7.989	7.989	7.989	7.989
28,000	8.404	8.404	8.404	8.404	8.404
30,000	8.807	8.807	8.807	8.807	8.807
35,000	9.776	9.776	9.776	9.776	9.776
40,000	10.720	10.720	10.720	10.719	10.719
45,000	11.691	11.691	11.690	11.685	11.678
50,000	12.756	12.756	12.755	12.734	12.701

**Table B.36** Internal partition function of  $Ar^{+4}$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	1.000	1.000	1.000	1.000	1.000
200	1.012	1.012	1.012	1.012	1.012
300	1.077	1.077	1.077	1.077	1.077
400	1.195	1.195	1.195	1.195	1.195
500	1.346	1.346	1.346	1.346	1.346
600	1.517	1.517	1.517	1.517	1.517
700	1.700	1.700	1.700	1.700	1.700
800	1.888	1.888	1.888	1.888	1.888
900	2.078	2.078	2.078	2.078	2.078
1000	2.268	2.268	2.268	2.268	2.268
1500	3.154	3.154	3.154	3.154	3.154
2000	3.892	3.892	3.892	3.892	3.892
2500	4.487	4.487	4.487	4.487	4.487
3000	4.970	4.970	4.970	4.970	4.970
3500	5.368	5.368	5.368	5.368	5.368
4000	5.703	5.703	5.703	5.703	5.703
4500	5.990	5.990	5.990	5.990	5.990
5000	6.242	6.242	6.242	6.242	6.242
6000	6.671	6.671	6.671	6.671	6.671
7000	7.034	7.034	7.034	7.034	7.034
8000	7.353	7.353	7.353	7.353	7.353
9000	7.641	7.641	7.641	7.641	7.641
10000	7.905	7.905	7.905	7.905	7.905
11000	8.149	8.149	8.149	8.149	8.149
12000	8.377	8.377	8.377	8.377	8.377
13000	8.590	8.590	8.590	8.590	8.590
14000	8.790	8.790	8.790	8.790	8.790
15000	8.979	8.979	8.979	8.979	8.979
16000	9.157	9.157	9.157	9.157	9.157
17000	9.327	9.327	9.327	9.327	9.327
18000	9.488	9.488	9.488	9.488	9.488
19000	9.641	9.641	9.641	9.641	9.641
20000	9.788	9.788	9.788	9.788	9.788
22000	10.065	10.065	10.065	10.065	10.065
24000	10.323	10.323	10.323	10.323	10.323
26000	10.567	10.567	10.567	10.567	10.567
28000	10.800	10.800	10.800	10.800	10.800
30000	11.026	11.026	11.026	11.026	11.026
35000	11.579	11.579	11.579	11.579	11.579
40000	12.139	12.139	12.139	12.139	12.139
45000	12.729	12.729	12.729	12.729	12.729
50000	13.366	13.366	13.366	13.366	13.366

## B.4 Selfconsistent Partition Functions of Atomic Species in Jupiter Atmosphere

**Table B.37** Internal partition function of  $H$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.000	2.000	2.000	2.000	2.000
200	2.000	2.000	2.000	2.000	2.000
300	2.000	2.000	2.000	2.000	2.000
400	2.000	2.000	2.000	2.000	2.000
500	2.000	2.000	2.000	2.000	2.000
600	2.000	2.000	2.000	2.000	2.000
700	2.000	2.000	2.000	2.000	2.000
800	2.000	2.000	2.000	2.000	2.000
900	2.000	2.000	2.000	2.000	2.000
1,000	2.000	2.000	2.000	2.000	2.000
1,500	2.000	2.000	2.000	2.000	2.000
2,000	2.000	2.000	2.000	2.000	2.000
2,500	2.000	2.000	2.000	2.000	2.000
3,000	2.000	2.000	2.000	2.000	2.000
3,500	2.000	2.000	2.000	2.000	2.000
4,000	2.000	2.000	2.000	2.000	2.000
4,500	2.000	2.000	2.000	2.000	2.000
5,000	2.000	2.000	2.000	2.000	2.000
6,000	2.000	2.000	2.000	2.000	2.000
7,000	2.000	2.000	2.000	2.000	2.000
8,000	2.000	2.000	2.000	2.000	2.000
9,000	2.001	2.000	2.000	2.000	2.000
10,000	2.003	2.001	2.000	2.000	2.000
11,000	2.014	2.005	2.002	2.001	2.000
12,000	2.042	2.013	2.005	2.002	2.001
13,000	2.127	2.030	2.011	2.005	2.003
14,000	2.328	2.070	2.022	2.009	2.006
15,000	2.757	2.146	2.044	2.018	2.011
16,000	3.585	2.322	2.068	2.026	2.015
17,000	5.069	2.572	2.119	2.044	2.024
18,000	7.562	3.093	2.243	2.071	2.038
19,000	11.529	3.728	2.381	2.108	2.040
20,000	17.562	4.975	2.570	2.159	2.057
22,000	33.846	8.884	3.416	2.310	2.106
24,000	64.303	16.090	4.544	2.543	2.177
26,000	113.016	28.212	7.108	3.197	2.273
28,000	173.160	47.204	9.825	3.809	2.398
30,000	269.420	67.715	15.712	4.589	2.552
35,000	609.149	192.913	36.505	9.190	3.722
40,000	1,142.980	371.747	73.552	14.390	4.875
45,000	1,891.330	574.449	132.056	27.130	6.287
50,000	2,864.220	896.095	217.103	37.351	11.248

**Table B.38** Internal partition function of *He* as a function of pressure and temperature

<i>T</i> (K)	<i>P</i> (bar)				
	10 <sup>-2</sup>	10 <sup>-1</sup>	1	10 <sup>1</sup>	10 <sup>2</sup>
100	1.000	1.000	1.000	1.000	1.000
200	1.000	1.000	1.000	1.000	1.000
300	1.000	1.000	1.000	1.000	1.000
400	1.000	1.000	1.000	1.000	1.000
500	1.000	1.000	1.000	1.000	1.000
600	1.000	1.000	1.000	1.000	1.000
700	1.000	1.000	1.000	1.000	1.000
800	1.000	1.000	1.000	1.000	1.000
900	1.000	1.000	1.000	1.000	1.000
1000	1.000	1.000	1.000	1.000	1.000
1500	1.000	1.000	1.000	1.000	1.000
2000	1.000	1.000	1.000	1.000	1.000
2500	1.000	1.000	1.000	1.000	1.000
3000	1.000	1.000	1.000	1.000	1.000
3500	1.000	1.000	1.000	1.000	1.000
4000	1.000	1.000	1.000	1.000	1.000
4500	1.000	1.000	1.000	1.000	1.000
5000	1.000	1.000	1.000	1.000	1.000
6000	1.000	1.000	1.000	1.000	1.000
7000	1.000	1.000	1.000	1.000	1.000
8000	1.000	1.000	1.000	1.000	1.000
9000	1.000	1.000	1.000	1.000	1.000
10000	1.000	1.000	1.000	1.000	1.000
11000	1.000	1.000	1.000	1.000	1.000
12000	1.000	1.000	1.000	1.000	1.000
13000	1.000	1.000	1.000	1.000	1.000
14000	1.000	1.000	1.000	1.000	1.000
15000	1.000	1.000	1.000	1.000	1.000
16000	1.001	1.000	1.000	1.000	1.000
17000	1.003	1.001	1.000	1.000	1.000
18000	1.009	1.002	1.000	1.000	1.000
19000	1.023	1.004	1.001	1.000	1.000
20000	1.053	1.010	1.002	1.001	1.000
22000	1.194	1.041	1.009	1.002	1.001
24000	1.614	1.137	1.025	1.006	1.002
26000	2.646	1.384	1.076	1.018	1.004
28000	4.601	1.942	1.165	1.039	1.009
30000	8.621	2.855	1.389	1.075	1.017
35000	32.750	10.919	2.793	1.379	1.093
40000	95.074	31.308	6.851	2.030	1.243
45000	222.978	67.850	16.128	3.961	1.523
50000	447.439	139.700	34.252	6.721	2.462

**Table B.39** Internal partition function of  $He^+$  as a function of pressure and temperature

$T$ (K)	$P$ (bar)				
	$10^{-2}$	$10^{-1}$	1	$10^1$	$10^2$
100	2.000	2.000	2.000	2.000	2.000
200	2.000	2.000	2.000	2.000	2.000
300	2.000	2.000	2.000	2.000	2.000
400	2.000	2.000	2.000	2.000	2.000
500	2.000	2.000	2.000	2.000	2.000
600	2.000	2.000	2.000	2.000	2.000
700	2.000	2.000	2.000	2.000	2.000
800	2.000	2.000	2.000	2.000	2.000
900	2.000	2.000	2.000	2.000	2.000
1,000	2.000	2.000	2.000	2.000	2.000
1,500	2.000	2.000	2.000	2.000	2.000
2,000	2.000	2.000	2.000	2.000	2.000
2,500	2.000	2.000	2.000	2.000	2.000
3,000	2.000	2.000	2.000	2.000	2.000
3,500	2.000	2.000	2.000	2.000	2.000
4,000	2.000	2.000	2.000	2.000	2.000
4,500	2.000	2.000	2.000	2.000	2.000
5,000	2.000	2.000	2.000	2.000	2.000
6,000	2.000	2.000	2.000	2.000	2.000
7,000	2.000	2.000	2.000	2.000	2.000
8,000	2.000	2.000	2.000	2.000	2.000
9,000	2.000	2.000	2.000	2.000	2.000
10,000	2.000	2.000	2.000	2.000	2.000
11,000	2.000	2.000	2.000	2.000	2.000
12,000	2.000	2.000	2.000	2.000	2.000
13,000	2.000	2.000	2.000	2.000	2.000
14,000	2.000	2.000	2.000	2.000	2.000
15,000	2.000	2.000	2.000	2.000	2.000
16,000	2.000	2.000	2.000	2.000	2.000
17,000	2.000	2.000	2.000	2.000	2.000
18,000	2.000	2.000	2.000	2.000	2.000
19,000	2.000	2.000	2.000	2.000	2.000
20,000	2.000	2.000	2.000	2.000	2.000
22,000	2.000	2.000	2.000	2.000	2.000
24,000	2.000	2.000	2.000	2.000	2.000
26,000	2.000	2.000	2.000	2.000	2.000
28,000	2.000	2.000	2.000	2.000	2.000
30,000	2.000	2.000	2.000	2.000	2.000
35,000	2.002	2.001	2.000	2.000	2.000
40,000	2.023	2.007	2.002	2.000	2.000
45,000	2.146	2.045	2.011	2.002	2.001
50,000	2.619	2.197	2.049	2.010	2.003

# Appendix C

## Constants

$a_0$	$0.529177249 \times 10^{-10}$	(m)	Bohr radius
$c$	299792458	(ms <sup>-1</sup> )	Speed of light
$e$	2.718281828		Neper number
$\epsilon_0$	$8.85415 \times 10^{-12}$	(C <sup>2</sup> m <sup>-1</sup> J <sup>-1</sup> )	Vacuum dielectric constant
$m_e$	$9.1093897 \times 10^{-31}$	(kg)	Electron mass
$m_p$	$1.67262158 \times 10^{-27}$	(kg)	Proton mass
AMU	$1.66053886 \times 10^{-27}$	(kg)	Atomic Mass Unit
$N_a$	$6.0221367 \times 10^{23}$	(mol <sup>-1</sup> )	Avogadro number
$h$	$6.6260755 \times 10^{-34}$	(Js)	Plank Constant
$\hbar = \frac{h}{2\pi}$	$1.05457266 \times 10^{-34}$	(Js)	Reduced Plank Constant
$k$	$1.380658 \times 10^{-23}$	(JK <sup>-1</sup> )	Boltzmann Constant
	$8.617386 \times 10^{-5}$	(eVK <sup>-1</sup> )	
	$6.950388 \times 10^{-1}$	(cm <sup>-1</sup> K <sup>-1</sup> )	
$I_H$	13.6	(eV)	Atomic hydrogen ionization potential
$q_e$	$1.6021773 \times 10^{-19}$	(C)	Electron charge
$R$	8.314510	(JK <sup>-1</sup> mol <sup>-1</sup> )	Ideal gas constant

### C.1 Conversion Factors

$$\text{cm}^{-1} = 1.239842447 \times 10^{-4} \text{ eV}$$

$$J = q_e \text{ eV}$$

$$R = N_a k$$

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