F.2 Degeneracy, Electronic States, Bond and Ionization Energies

The degeneracy and electronic states of the atomic species needed for the partition function computations can be determined by using the NIST atomic spectroscopy data base which gives electronic orbital configurations, spectroscopic terms and energy levels for neutral species and the first ion. See p. 69-73, particularly Table 3.2 and the following paragraph in Boyd and Schwartzentruber (2017) to translate the spectroscopic term symbols into degeneracy factors. The values of enthalpy at 0 K are from Table B1 in McBride et al. (2002). This is used to compute the heat of reaction for the ionized species at 0 K. The tabulated bond dissociation energies are from deB Darwent (1970). Except for NO which is from Table "Bond Dissociation Energies" in Rumble (2018). Values of D^o are for 0 K; D^o(0 K) = D^o(298.15 K) - 3.7181 J/mol-K

Table F.4: Degeneracy factors, ionization, enthalpy at zero temperature and dissociation energies for selected species.

	g	I (eV)	$H^\circ(0)$ (kJ/mol)	D° (kJ/mol)
e^-	2	-	-6.197	-
N	4	14.53	466.483	-
N^+	9	29.60	1875.011	-
N_2	1	15.57	-8.670	941.636
N_2^+	2		1500.837	-
O	9	13.61	242.450	-
O^+	4	35.12	1562.590	-
O_2	3	12.07	-8.680	493.58
O_2^+	4		1162.517	-
NO	4	9.264	82.092	626.841
NO^+	1		982.140	-
Ar	1	15.76	-6.197	-
Ar^+	6	27.63	1520.572	-
H	2	13.60	211.8	-
H^+	1	-	1530.	-

Appendix G

Constants and Conversions

G.1 Fundamental Physical Constants

c_o	speed of light in a vacuum	2.99792×10^{8}	$\mathrm{m\cdot s^{-1}}$
ϵ_o	permittivity of the vacuum	8.85419×10^{-12}	$\mathrm{F\cdot m^{-1}}$
μ_o	permeability of the vacuum	$4\pi\times10^{-7}$	$\mathrm{N\cdot A^{-2}}$
h	Planck constant	6.62607×10^{-34}	$\mathrm{J\cdot s}$
k	Boltzmann constant	1.38065×10^{-23}	$\mathrm{J\cdot K^{-1}}$
N_o	Avogadro number	6.02214×10^{23}	$\mathrm{molecules\cdot mol^{-1}}$
e	charge on electron	1.60218×10^{-19}	C
amu	atomic mass unit	1.66054×10^{-27}	kg
m_e	electron mass	9.10938×10^{-31}	kg
m_p	proton mass	1.67262×10^{-27}	kg
G	universal gravitational constant	6.67430×10^{-11}	$\mathrm{m^3\cdot kg^{-1}\cdot s^{-2}}$
σ	Stefan-Boltzmann constant	5.67037×10^{-8}	$\mathrm{W\cdot m^{-2}K^{-4}}$

Consistent with the 2018 CODATA adjustment of the fundamental physical constants. For the most recent values, see NIST Reference on Units and Uncertainty.

G.2 Gases

Universal Gas Constant

$\tilde{R}$	8314.462	$\mathrm{J\cdot kmol^{-1}\cdot K^{-1}}$
$\tilde{R}$	8.314462	$\mathrm{J\cdot mol^{-1}\cdot K^{-1}}$
$\tilde{R}$	82.0575	$\mathrm{cm^3\cdot atm\cdot mol^{-1}\cdot K^{-1}}$
$\tilde{R}$	1.9872	$\mathrm{cal\cdot mol^{-1}\cdot K^{-1}}$

Gas Properties at 273.15 K and 1 atm

pressure	101325	Pa
volume of 1 kmol	22.414	$\mathrm{m^3}$
number of molecules per unit volume	2.25×10^{25}	$\mathrm{m^{-3}}$
collision frequency at 273.15 K and 1 atm	4.3×10^{9}	$\mathrm{s^{-1}}$
mean free path in N_2 at 273.15 K and 1 atm	74	nm

G.3 Our Atmosphere

	composition (mol fractions)		
		0.7808	N_2
		0.2095	O_2
		0.0093	Ar
		0.0004	CO_2
Sea level			
P	pressure	1.01325×10^5	Pa
ρ	density	1.225	kg/m^3
T	temperature	288.15	K
c	sound speed	340.29	m/s
R	gas constant	287.05	m^2/s^2-K
W	molar mass	28.96	kg/kmol
μ	viscosity (absolute)	1.79×10^{-5}	kg/m-s
k	thermal conductivity	2.54×10^{-3}	W/m-K
c_p	heat capacity	1.0	kJ/kg-K
30 kft			
P	pressure	3.014×10^4	Pa
ρ	density	0.458	kg/m^3
T	temperature	228.7	K
c	sound speed	303.2	m/s

Based on the U.S. Standard Atmosphere, Minzer et al. (1975).

G.4 Unit Conversions

	Engineering	
2.54 cm	$\equiv$	1.00 in
1 m	$\equiv$	3.2808 ft
0.3048 ft	$\equiv$	1 m
1 lb (force)	$\equiv$	4.452 N
1 lb (mass)	$\equiv$	0.454 kg
1 btu	$\equiv$	1055.06 J
1 hp	$\equiv$	745.7 W
1 hp	$\equiv$	550 ft-$\mathrm{lb}_f \cdot \mathrm{s}^{-1}$
1 mile (land)	$\equiv$	1.609 km
1 mph	$\equiv$	0.447 $\mathrm{m} \cdot \mathrm{s}^{-1}$
1 mile (nautical)	$\equiv$	1.852 km
	mechanical equivalent of heat	
1 cal	$\equiv$	4.184 J
	Molecular	
1 eV	$\equiv$	1.602176×10^{-19} J
1 eV $\cdot$molecule^{-1}	$\equiv$	96.485 $\mathrm{kJ} \cdot \mathrm{mol}^{-1}$
1 eV	$\equiv$	11604.52 K
1 cm^{-1}	$\equiv$	1.43877 K
1 cm^{-1}	$\equiv$	11.9627 $\mathrm{J} \cdot \mathrm{mol}^{-1}$
1 $\mathrm{kJ} \cdot \mathrm{mol}^{-1}$	$\equiv$	120.272 K

For on-line units conversions, see NIST Links.