



TABLE 4.1 PARTITION FUNCTIONS FOR DIFFERENT TYPES OF MOTION

| Motion | Degrees of freedom | Partition function | Order of magnitude |
|----------------------------------|--------------------|--|----------------------------------|
| Translation | 3 | $\frac{(2\pi mkT)^{3/2}}{h^3}$ (per unit volume) | $10^{31}-10^{32} \text{ m}^{-3}$ |
| Rotation (linear molecule) | 2 | $\frac{8\pi^2IkT}{\sigma h^2}$ | $10-10^2$ |
| Rotation (nonlinear molecule) | 3 | $\frac{8\pi^2(8\pi^3I_A I_B I_C)^{1/2}(kT)^{3/2}}{\sigma h^3}$ | 10^2-10^3 |
| Vibration (per normal mode) | 1 | $\frac{1}{1 - e^{-h\nu/kT}}$ | 1-10 |
| Free internal rotation | 1 | $\frac{(8\pi^2I'kT)^{1/2}}{h}$ | 1-10 |

where m = mass of molecule
 I = moment of inertia for linear molecule
 $I_A, I_B,$ and I_C = moments of inertia for a nonlinear molecule about three axes at right angles to one another
 I' = moment of inertia for internal rotation
 ν = normal-mode vibrational frequency
 k = Boltzmann constant
 h = Planck constant
 T = absolute temperature
 σ = symmetry number^a

It is useful to remember that the power to which h appears is equal to the number of degrees of freedom.

^a As discussed in the text (Section 4.5.4), symmetry numbers are used in the calculation of equilibrium constants, but for rates an alternative procedure is recommended.