FUNÇÕES DE PARTIÇÃO

TABLE 4.1 PARTITION FUNCTIONS FOR DIFFERENT TYPES OF MOTION

Motion	Degrees of freedom	Partition function	Order of magnitude
Translation	3	$\frac{(2\pi m\mathbf{k}T)^{3/2}}{h^3}$ (per unit volume)	10^{31}–10^{32} m^{-3}
Rotation (linear molecule)	2	$\frac{8\pi^2 I\mathbf{k}T}{\sigma h^2}$	10–10^2
Rotation (nonlinear molecule)	3	$\frac{8\pi^2(8\pi^3 I_A I_B I_C)^{1/2}(\mathbf{k}T)^{3/2}}{\sigma h^3}$	10^2–10^3
Vibration (per normal mode)	1	$\frac{1}{1-e^{-h\nu/\mathbf{k}T}}$	1–10
Free internal rotation	1	$\frac{(8\pi^2 I'\mathbf{k}T)^{1/2}}{h}$	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
$\mathbf{k}$ = 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.

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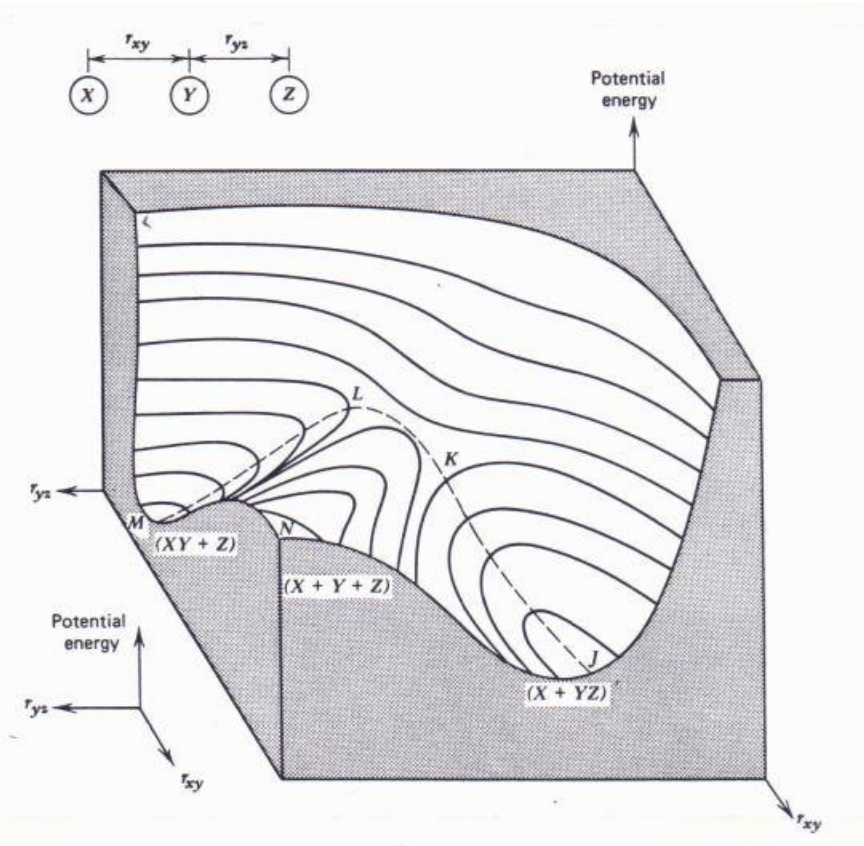

r_{xy}
r_{yz}
X
Y
Z
Potential energy
L
K
M
N
J
(XY + Z)
(X + Y + Z)
(X + YZ)
r_{yz}
Potential energy
r_{yz}
r_{xy}
r_{xy}