

### Useful Equation

Units  $1 \text{ mol} = 6.023 \times 10^{23}$ ,  $1 \text{ mm} = 10^{-3} \text{ m}$ ,  $1 \mu\text{m} = 10^{-6} \text{ m}$ ,  $1 \text{ nm} = 10^{-9} \text{ m}$ ,  $1 \text{ pm} = 10^{-12} \text{ m}$ ,  $1 \text{ fm} = 10^{-15} \text{ m}$ , **molar concentration**  $1 \text{ M} = \frac{1 \text{ mol}}{L}$ , with  $1 \text{ L} = 10^{-3} \text{ m}^3$ ,  $1 \text{ M} = 6.023 \times$

$10^{26} \text{ m}^{-3}$ . 1 molecule in a box size of  $1 \text{ nm}^3 \rightarrow \frac{1 \div 6.023 \times 10^{23} \text{ mol}^{-1}}{1 \text{ nm}^3 \times 10^{-27} \text{ m}^3 \cdot \text{nm}^{-3} \times 10^3 \text{ L} \cdot \text{m}^{-3}} = 1.6 \frac{\text{mol}}{\text{L}} = 1.6 \text{ M}$ .

**Algebra:**  $\ln(xy) = \ln x + \ln y$ ;  $\ln\left(\frac{x}{y}\right) = \ln x - \ln y$ ;  $\ln x^n = n \ln x$ ;  $e = 2.71828$ ;  $\ln e = 1$ ;  $2^x =$

$10^{0.301x}$ . **Calculus:**  $\frac{d(e^{ax})}{dx} = ae^{ax}$ ;  $\frac{d(e^{af(x)})}{dx} = a \frac{df(x)}{dx} e^{af(x)}$ ;  $\frac{d(\ln ax)}{dx} = \frac{1}{x}$ ;  $\frac{d(\ln af(x))}{dx} = \frac{1}{f(x)} \frac{df}{dx}$ .

**Thermodynamics:**  $PV = Nk_B T$ ,  $k_B = 1.381 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$ , 1<sup>st</sup> law of Thermodynamics:

$dE = TdS - PdV + \mu dN \rightarrow dS = \frac{1}{T} dE + \frac{P}{T} dV - \frac{\mu}{T} dN$ , entropy  $S(E, V, N) \rightarrow dS =$

$\left(\frac{\partial S}{\partial E}\right)_{V,N} dE + \left(\frac{\partial S}{\partial V}\right)_{E,N} dV - \left(\frac{\partial S}{\partial N}\right)_{E,V} dN \rightarrow \left(\frac{\partial S}{\partial E}\right)_{V,N} = \frac{1}{T}$ ;  $\left(\frac{\partial S}{\partial V}\right)_{E,N} = \frac{P}{T}$ ;  $\left(\frac{\partial S}{\partial N}\right)_{E,V} = -\frac{\mu}{T}$

**Pressure:**  $1 \text{ atm} = 1.01325 \times 10^5 \frac{\text{N}}{\text{m}^2} = 1.01325 \times 10^5 \text{ Pa}$ ;  $1 \text{ mm Hg} = 133 \text{ Pa}$ ;  $760 \text{ mm Hg} = 1$

**atm.** **Osmotic Pressure**  $P = n_{\text{sol}} k_B T$ ,  $n_{\text{sol}}$  is solute number concentration. **ideal gas, Sackur-**

**Tetrode equation:**  $S = Nk_B \left[ \ln \left\{ \left( \frac{V}{N} \right) \left( \frac{4\pi m E}{3N h^2} \right)^{3/2} \right\} + \frac{5}{2} \right] \rightarrow PV = Nk_B T$ , equipartition theorem,

$E = \frac{3}{2} Nk_B T$ . Thermodynamic definition of entropy,  $\Delta S = \frac{\text{heat}}{T} = \frac{Q}{T} \rightarrow$  for gas/liquid  $dS = S_{\text{gas}} -$

$S_{\text{liquid}} = \frac{Q_{\text{vaporization}}}{T}$ , and using **Sackur-Tetrode**,  $\frac{W_{\text{gas}}}{W_{\text{liquid}}} \sim \left( \frac{V_{\text{gas}}}{V_{\text{liquid}}} \right)^N$ . Also  $PV = nRT$ ,  $n$  is

number of mole,  $R = 8.314 \frac{\text{J}}{\text{K} \cdot \text{mol}}$ . **Fluid drag force**,  $f = v\zeta$ ,  $\zeta = 6\pi\eta R$ , for example viscosity

of water,  $\eta = 10^{-3} \text{ Pa} \cdot \text{s} = 10^{-3} \frac{\text{kg}}{\text{m} \cdot \text{s}}$ , also power = force times speed,  $P = fv$ . Fluctuation-

Dissipation  $D = \frac{k_B T}{\zeta}$ . **Energy:** ATP hydrolysis, *in vitro*  $\Delta G \sim -32 \frac{\text{kJ}}{\text{mol}}$ , *in vivo*  $\Delta G \sim -54 \frac{\text{kJ}}{\text{mol}}$ .

**Stirling Approximation:** large  $N$ ,  $\ln N! \sim N \ln N - N$ , or more exact  $N! \sim N^N e^{-N} (2\pi N)^{1/2}$ .

**Receptor-Ligand Binding:**  $L + R \leftrightarrow LR$ ,  $k_d = \frac{[L][R]}{[LR]}$ ,  $P_{\text{bound}} = \frac{[LR]}{[R] + [LR]}$  or for lattice model,

$P_{\text{bound}} = \frac{(c/c_0)e^{-\beta\Delta\varepsilon}}{1 + (c/c_0)e^{-\beta\Delta\varepsilon}}$ ,  $c = [L]$ , reference concentration  $c_0 = \frac{1}{V_{\text{box}}}$ , with  $k_d = \frac{1}{V_{\text{box}}} e^{\beta\Delta\varepsilon}$ . **Hill**

**Function**,  $P_{\text{bound}} = \frac{([L]/k_d)^n}{1 + ([L]/k_d)^n}$ ,  $n$  is the order of the Hill Function. For two ligands 1 and 2, with

concentration  $[L]_1$  and  $[L]_2$  of order  $n_1$  and  $n_2$ , respectively,  $P_{\text{bound},1} = \frac{([L]_1/k_{d1})^{n_1}}{1 + ([L]_1/k_{d1})^{n_1} + ([L]_2/k_{d2})^{n_2}}$ ,

and similar for  $P_{\text{bound},2}$ , with  $k_{d1}$  and  $k_{d2}$ , the respective dissociation constants.

**Polymer/DNA:**  $\langle R_{ee}^2 \rangle = Na^2$ ,  $N$  is number of Kuhn segments,  $a$  is the length of a Kuhn

segment,  $a = 300L_{bp}$ , where  $L_p = \frac{1}{3} \text{ nm}$  is the average length of one basepair (bp),  $a = 100 \text{ nm}$ .

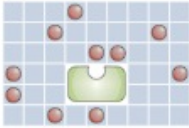

$\sqrt{\langle R_G^2 \rangle} = \sqrt{\frac{L\xi_p}{3}}$ , with the persistent length  $\xi_p = \frac{a}{2} = 50 \text{ nm}$ . **Free Polymer:**  $P(r) =$

$\left( \frac{3}{2\pi Na^2} \right)^{3/2} 4\pi r^2 e^{-\frac{3r^2}{2Na^2}}$ ; **Tethered polymer:**  $P(r) = \left( \frac{3}{2\pi Na^2} \right)^{1/2} \frac{r}{R} \left( e^{-\frac{3(r-R)^2}{2Na^2}} + e^{-\frac{3(r+R)^2}{2Na^2}} \right)$ .

**partition function**  $Z = \sum_{\varepsilon} g \exp(-\beta\varepsilon)$ , with summation over all microstates, and  $\varepsilon$  is the energy of a group of microstates with the same energy, and  $g(\varepsilon)$  is the multiplicity or the number of microstates that has the energy  $\varepsilon$ . The probability that a microstate with energy  $\varepsilon$  is

occupied is simply  $P(\varepsilon) = \frac{g(\varepsilon) \exp(-\beta\varepsilon)}{Z}$ . Average Energy  $\langle E \rangle = \sum_{\varepsilon} \varepsilon P(\varepsilon) = \frac{\sum_{\varepsilon} \varepsilon g(\varepsilon)}{Z}$

More Data: 1 Dalton (Da) =  $1.6 \times 10^{-27} \text{ kg}$ ; 1 protein  $\sim 300 \text{ aa}$ ; 1 Hemoglobin mass  $\sim 64\,000 \text{ Da}$ , diameter 5.8 nm. E. Coli  $\sim 5400 \text{ genes}$ ,  $5.4 \times 10^6 \text{ bp}$ .

STATE	ENERGY	MULTIPLICITY	WEIGHT
(A) 	$Le_{\text{sol}}$	$\frac{\Omega!}{L!(\Omega-L)!} \approx \frac{\Omega^L}{L!}$	$\frac{\Omega^L}{L!} e^{-\beta Le_{\text{sol}}}$
(B) 	$(L-1)e_{\text{sol}} + e_{\text{b}}$	$\frac{\Omega!}{(L-1)!(\Omega-L+1)!} = \frac{\Omega^{L-1}}{(L-1)!}$	$\frac{\Omega^{L-1}}{(L-1)!} e^{-\beta[(L-1)e_{\text{sol}} + e_{\text{b}}]}$

The left figure shows the binding model when the ligands are **indistinguishable**. For example, if all ligands are on the lattice (no binding), the multiplicity of  $L$  ligands on  $\Omega$  lattice sites is

$$\text{multiplicity} = \frac{\Omega!}{L!(\Omega-L)!}$$

The  $L!$  is needed to correct for the overcounting. On the other hands if the ligands are **distinguishable** then the multiplicity of arranging  $L$  ligands on  $\Omega$  lattice sites is

$$\text{multiplicity} = \Omega(\Omega-1)(\Omega-2) \cdots (\Omega-L+1) = \frac{\Omega!}{(\Omega-L)!}$$