

Biology 3550: Physical Principles in Biology

Fall Semester - 2018

Important Equations for the Final Exam

The following are important equations that have been introduced during the semester and might (or might not) be useful for the final exam. You are encouraged to review these equations, their meaning and applications as you study for the exam. These equations will also be provided on the exam, but without all of the explanations and variable definitions given here.

This list does not include every possible relationship that you might be expected to know. You should know, for instance, equations for calculating the areas or volumes of simple shapes; for calculating concentrations; and the basic rules of probability, such as when to add or multiply probabilities, how to calculate expected values and how to interpret continuous probability distribution functions.

Spend your time thinking and solving problems, not memorizing!

Derived SI units

- Force (newton or N)

$$1 \text{ N} = 1 \text{ kg} \cdot \text{m} \cdot \text{s}^{-2}$$

- Energy or work (joule or J)

$$1 \text{ J} = 1 \text{ N} \cdot \text{m} = 1 \text{ kg} \cdot \text{m}^2 \cdot \text{s}^{-2}$$

Conversion factors

- L to cubic meters

$$1 \text{ L} = 10^{-3} \text{ m}^3$$

Constants

- Avogadro's number, $N_A = 6.02 \times 10^{23}$
- Gas constant: $R = 8.314 \text{ L} \cdot \text{kPa} \cdot \text{K}^{-1} \text{mol}^{-1} = 8.314 \text{ J} \cdot \text{K}^{-1} \text{mol}^{-1}$
- Boltzmann constant: $k = 1.38 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$

Probability

- Binomial coefficients (the number of ways to choose either k unlabeled items or k labeled items in a unique order), from a collection of n .

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

- The Gaussian (normal) probability distribution function for a random variable x with mean μ and standard deviation σ

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/(2\sigma^2)}$$

Random walks in one, two or three dimensions

- Parameters:

δ = fixed step length or root-mean-square length of random step lengths

n = number of steps

δ_i = positive or negative displacement for a single step, i

$\langle \delta_i \rangle$ = mean displacement, over many steps

$\langle \delta_i^2 \rangle$ = mean-square displacement, over many steps

- End-to-end distance, r

$$\langle r^2 \rangle = n \langle \delta_i^2 \rangle$$

$$\text{RMS}(r) = \sqrt{\langle r^2 \rangle}$$

- Mean-square net displacement along the x -axis in a two-dimensional random walk, if $\langle \delta_i \rangle = 0$.

$$\langle x^2 \rangle = n\delta^2/2$$

- Mean-square net displacement along the x -axis in a three-dimensional random walk, if $\langle \delta_i \rangle = 0$.

$$\langle x^2 \rangle = n\delta^2/3$$

Diffusion

- The diffusion coefficient, D

$$D = \frac{\delta_x^2}{2\tau}$$

where τ is the average time interval between direction changes of the diffusing molecule, and δ_x is the root-mean-square displacement along the x -direction between direction changes.

- Fick's first law:

$$J = -D \frac{dC}{dx}$$

where J is the flux (in moles or molecules per unit time per unit area), and dC/dx is the derivative of concentration with respect to x .

- Fick's second law:

$$\frac{dC}{dt} = D \frac{d^2C}{dx^2}$$

where dC/dt is the derivative of concentration with respect to time and d^2C/dx^2 is the second derivative of concentration with respect to x .

- Mean-square displacement along one direction due to diffusion:

$$\begin{aligned}\langle x^2 \rangle &= n\delta_x^2 = (t/\tau)\delta_x^2 \\ &= 2Dt\end{aligned}$$

where n is the number of random walk steps, t is the time and τ is the time interval between direction changes.

Kinetic energy and molecular motion

- Kinetic energy, in the x -direction, of an object with mass m and velocity v

$$E_{k,x} = mv^2/2$$

- Root-mean-square thermal kinetic energy, in the x -direction, of molecules of mass m at temperature T

$$\text{RMS}(E_{k,x}) = kT/2$$

- The Stokes-Einstein equation for calculating the diffusion coefficient for a spherical particle:

$$D = \frac{kT}{6\pi\eta r}$$

where η is the viscosity, in units of $\text{N} \cdot \text{sm}^{-3}$, and r is the sphere radius.

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- RMS velocity of molecules of mass m at temperature T

$$v = \sqrt{kT/m}$$

- The Stokes-Einstein equation for calculating the diffusion coefficient for a spherical particle:

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where η is the viscosity, in units of $\text{N} \cdot \text{s} \cdot \text{m}^{-3}$, and r is the sphere radius.

Thermodynamics

- Δf :

By convention, the change in a state function, f , for a process converting state 1 to state 2 is defined as the value of the state function for state 2 minus the value for state 1:

$$\Delta f = f_2 - f_1$$

- The first law of thermodynamics:

$$\Delta E = q + w$$

where ΔE is the change in internal energy of the system, q is the heat absorbed by the system and w is the work done on the system during a defined process or reaction.

- The classical definition for the change in the entropy of a system during a process at constant temperature:

$$\Delta S_{\text{sys}} = \frac{q_{\text{rev}}}{T}$$

where q_{rev} is the heat absorbed by the system for the reversible process connecting the beginning and ending states, and T is the absolute temperature.

- The classical definition for the change in the entropy of the surroundings during a process at constant temperature:

$$\Delta S_{\text{surr}} = -\frac{q}{T}$$

where q is the heat absorbed by the system during a specified process connecting the two states. ΔS_{surr} , is *not* a state function and depends on the particular path taken between the two states.

- The second law of thermodynamics:

The second law states that the total entropy of the universe, defined as

$$\Delta S_{\text{univ}} = \Delta S_{\text{surr}} + \Delta S_{\text{sys}}$$

increases for a spontaneous (favorable) process.

- The statistical (Boltzmann) definition of the entropy of a system:

$$S_{\text{sys}} = k \ln \Omega$$

where k is Boltzmann's constant and Ω is the total number of equal-energy microstates making up the system. The entropy calculated using this equation corresponds to a single copy of the defined system, and Ω represents the number of ways of arranging the various components of the system, such as molecules in a gas or units within a single molecule (such as amino-acid residues in a protein).

- The entropy change for the expansion or compression of an ideal gas:

$$\Delta S_{\text{sys}} = nR \ln \frac{V_2}{V_1}$$

where n is the number of moles, R is the gas constant, and V_1 and V_2 are the initial and final volumes of the gas. The entropy change can also be expressed in terms of the concentration of gas molecules and the beginning and end of the process:

$$\Delta S_{\text{sys}} = nR \ln \frac{C_1}{C_2}$$

This equation is also used as an approximation for calculating the entropy change due to a change in concentration of molecules in solution.

- Enthalpy, a state function:

$$H = E + PV$$

where E is the internal energy, P is the pressure and V is the volume of the system. The change in enthalpy for a process is the heat absorbed by the system in converting the system from state 1 to state 2 at constant pressure.

$$\Delta H = q_p$$

If there is no change in volume during the process at constant pressure, or other work performed on or by the system, $\Delta H = \Delta E$.

- The Helmholtz free energy:

$$F = E - TS_{\text{sys}}$$

For a process at constant temperature, the change in F is:

$$\Delta F = \Delta E - T\Delta S_{\text{sys}}$$

ΔF is also equal to the work done on the system during the reversible conversion of one state to another. If the process is favorable in the absence of work, then ΔF is negative, and $-\Delta F$ represents the maximum amount of work that can be done by the process. If the process is unfavorable, then ΔF is positive and represents the minimum amount of work required to drive the process forward.

- The Gibbs free energy:

$$G = H - TS_{\text{sys}}$$

For a process at constant temperature, the change in G is:

$$\Delta G = \Delta H - T\Delta S_{\text{sys}}$$

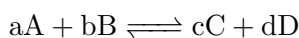
The Gibbs and Helmholtz free energy changes for a process are related to each other according to:

$$\begin{aligned} \Delta G &= \Delta F - w_p \\ &= w_{\text{rev}} - w_p \end{aligned}$$

where w_p is the work absorbed by converting state 1 to state 2 at constant pressure. If the process at constant pressure does not involve a volume change, then $w_p = 0$ and $\Delta G = \Delta F$. Because the volume changes for most biochemical processes are quite small, ΔG can be interpreted as the negative of the maximum work that can be obtained from a favorable process or, for an unfavorable process, the minimum amount of work required to drive the process forward.

- Reaction quotient, Q :

For the chemical reaction of the form:



The reaction quotient, for a given set of reactant and product concentrations is defined as:

$$Q = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$

- Equilibrium constant:

When the the reaction defined above is at equilibrium, the concentrations of reactants and products satisfy the expression:

$$K_{\text{eq}} = \frac{[C]_{\text{eq}}^c [D]_{\text{eq}}^d}{[A]_{\text{eq}}^a [B]_{\text{eq}}^b}$$

where K_{eq} is the equilibrium constant for the reaction, which typically depends on temperature and other solution conditions (sometimes including the concentrations of other molecules and ions in the solution).

- Standard free energy change:

The free energy change for a reaction at standard state concentrations (usually 1 M concentration for solutes and 1 atm pressure for gasses) is defined as ΔG° and is related to the equilibrium constant according to:

$$\Delta G^\circ = -RT \ln K_{\text{eq}}$$

where R is the gas constant and T is the temperature. Note that the units of concentration used to define the equilibrium constant must be the same as those defining the standard state for ΔG° .

- Free energy change when the concentrations are different from the standard state:

For any set of reactant concentrations, the free energy change for the reaction is:

$$\Delta G = \Delta G^\circ + RT \ln Q$$

Where Q is the reaction quotient defined above. Note that when the system is at equilibrium, $Q = K_{\text{eq}}$, and $\Delta G = 0$, meaning that no work can be obtained by the system. When the reactants and products are at their standard state concentrations $\Delta G = \Delta G^\circ$.

The value of ΔG at a given set of concentrations represents the free energy change for converting a mole of reactants into products, assuming that the concentrations of reactants and products don't actually change. This idealized situation would prevail if the volume were infinitely large.