Name Key

Chem 352 - Spring 2018
Quiz 1

$R = 8.314\ J/(mol \cdot K) = 0.08206\ (L \cdot atm)/(mol \cdot K)$

1. One of the reactions in the gluconeogenesis pathway, an *anabolic* metabolic pathway that leads to the synthesis of glucose, involves the hydration of *phosphoenolpyruvate* to form *2-phosphoglycerate*.

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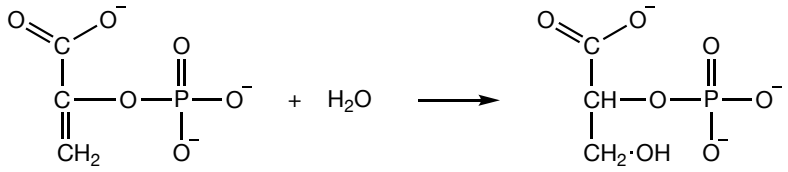


phosphoenolpyruvate 2-phosphoglycerate

a. Under standard state conditions at 25°C, the equilibrium constant for this reaction is $K_{eq} = 2.07$. Is this reaction favorable (spontaneous) at standard state conditions?
(Y/N?) Y
Explain: There are two ways to approach answering this question. You can either analyze K_{eq} directly, or use it to calculate $\Delta G°$, which is what you are asked to do below. Analyzing K_{eq}, since K_{eq} is greater than 1, it tells us that at equilibrium there will be more products than reactants, so starting at the standard state, where all the concentrations (except H_2O) are equal to 1 M, we expect the reaction to move spontaneously to the right, as written, in order to reach equilibrium.

(4 pts)

b. Determine the standard free energy change, $\Delta G°'$, for this reaction at 25°C.

$$\Delta G° = -RT\ln(K_{eq}) =$$
$$= -\left(8.314 \times 10^{-3}\ \frac{kcal}{mol \cdot K}\right)(273.15 + 25\ K)\ln(2.07)$$
$$= -1.80\ kcal$$

(4 pts)

Since $\Delta G°$ is less than 0, this confirms our analysis above that the reaction is favorable under standard state conditions

c. If the cellular concentrations of *phosphoenolpyruvate* and *2-phosphoglycerate*, are 1.2 mM and 5.1mM, respectively, is this reaction favorable under conditions found in a cell at 25°C (Y/N)? N
Explain:

$$\Delta G = \Delta G° + RT\ln\left(\frac{[\text{2-phosphoglycerate}]}{[\text{phosphoenolpyruvate}]}\right) =$$
$$= -1.80\ kcal + \left(8.314 \times 10^{-3}\ \frac{kcal}{mol \cdot K}\right)(273.15 + 25\ K)\ln\left(\frac{5.1 \times 10^{-3}\ M}{1.2 \times 10^{-3}\ M}\right)$$
$$= -1.80\ kcal + 3.59\ kcal$$
$$= 1.79\ kcal$$

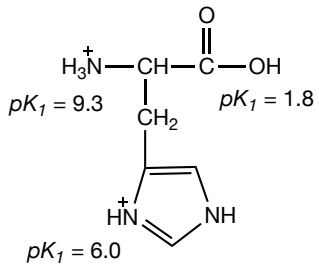
(4 pts)

Since ΔG is greater than 0 under conditions found in the cell, the reaction is unfavorable as written.

d. What is *anabolism*? The term anabolism is used to describe collectively the metabolic pathways that are used to synthesize larger molecules from smaller ones. These pathways also usually require a source of energy to drive them along.

(3 pts)

2. To the right is shown the structural formula for the amino acid histidine. Histidine contains three ionizable groups; the structure shown has all three of these groups in their protonated, acid form. The pK_a values for these three acids are indicated in the figure.



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a. What is the expected *pH* for a 50 mM solution of histidine in its fully protonated form? It is the ionizable group which is the strongest acid and has the lowest pK_a the will most greatly influence the *pH* of the fully protonated form of histidine in an aqueous solution. The $[H^{+}]$ of a weak acid solution is approximately equation to $\sqrt{K_a C_a}$, where K_a is the acid dissociation for the weak acid, and C_a is its concentration.

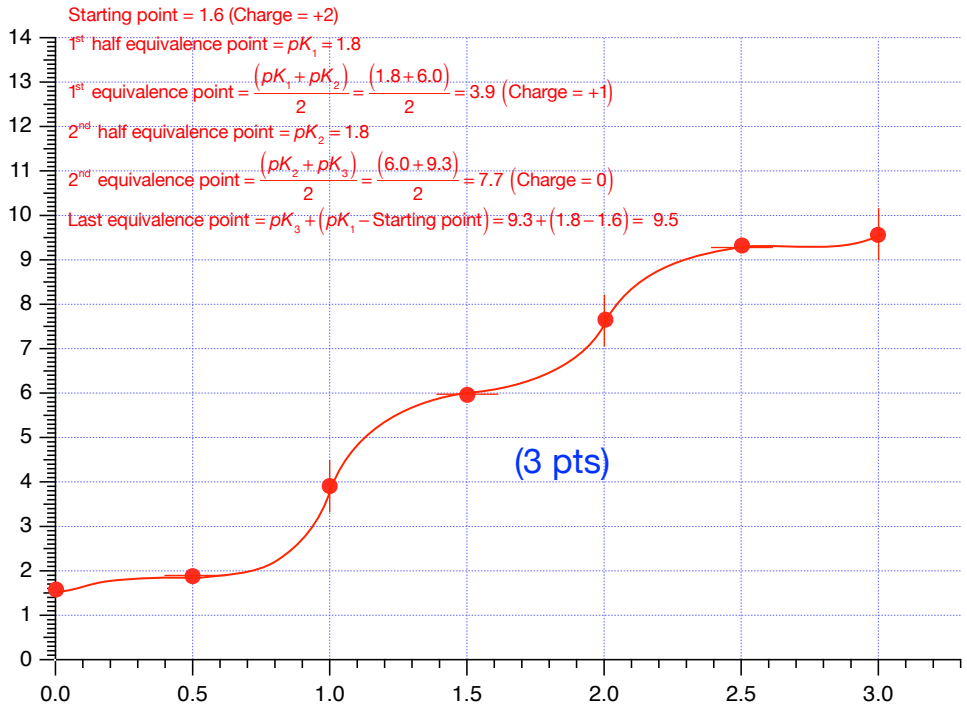
(3 pts)

$$[H^+] \approx \sqrt{K_a C_a}$$
$$\approx \sqrt{10^{-pK_1} C_a} \approx \sqrt{10^{-1.8}(50\text{x}10^{-3}\text{M})}$$
$$\approx 2.82 \text{ x } 10^{-2}\text{M}$$

histidine

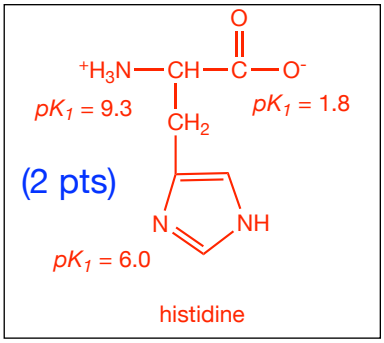
$$pH = -\log([H^+])$$
$$= -\log(2.82\text{x}10^{-2}\text{M})$$
$$= 1.55$$

b. Sketch the titration curve for a 50 mM solution of histidine. Be sure to properly label the axes.



c. What is the isoelectric *pH* for histidine? *pI* = 7.7 (2 pts)

d. Draw the structure for the predominant species of histidine that exists at its isoelectric *pH*. The isoelectric point is the equivalence point where the net charge on the histidine is 0. This comes at the second equivalence point where the α-carboxyl group (pK_1=1.8) and the side chain imidazole group (pK_2=6.0) have been converted to their conjugate base forms, but the α-amino group (pK_3) is still in its acid form.



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