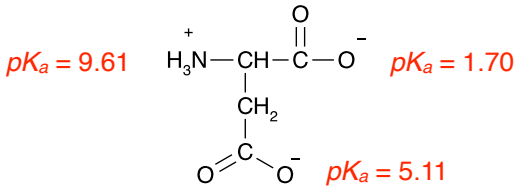
Name _____

# Chem 352 - Fall 2013
# Quiz 1 (Take home portion)

*R* = 8.314 *J/(mol•K)* = 0.08206 *(L•atm)/(mol•K)*

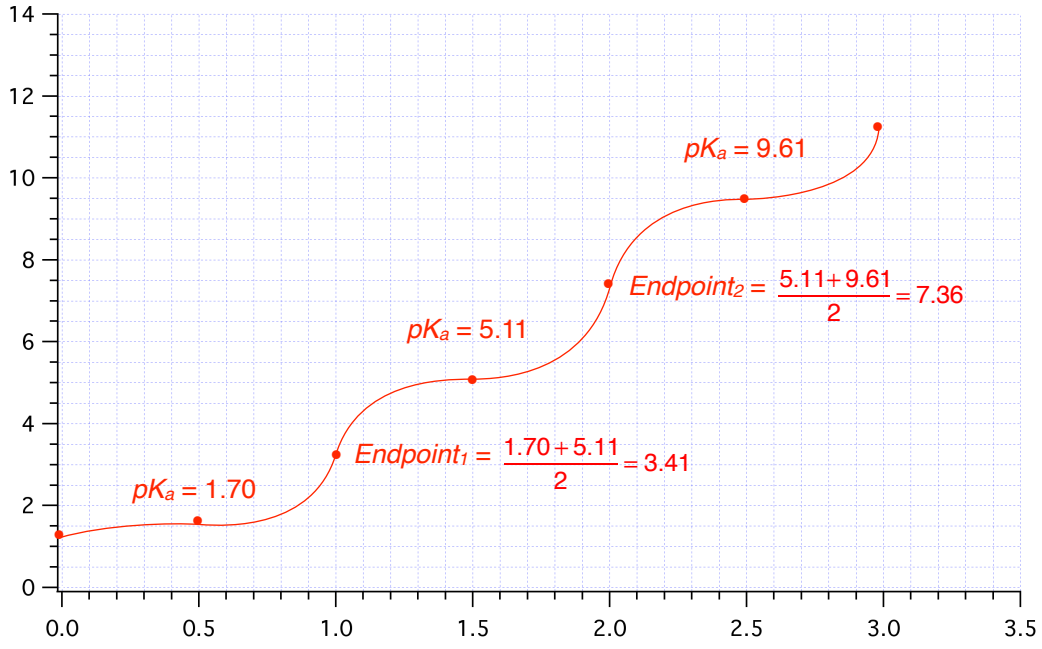
1. Aspartic acid is one of the 20 common amino acids and has a side chain with an acidic carboxylic acid group. The structure for aspartic acid in its partially protonated state is shown below:




   a. Use MarvinSketch to predict the $pK_a$ values for each of the ionizable groups of aspartic acid. (After drawing the structure, select "Calculations->Protonation->pKa)

   b. Draw, in order, the ionic species formed upon titration of aspartic acid from *pH* 0.0 to *pH* 10.0.

   c. Sketch the titration curve for aspartic acid as *pH vs. equivalents of base added*. You can check your work by selecting "Calculations->Protonation->Isoelectric point", MarvinSketch will create a plot of *net charge vs pH*, which is essentially the *x* <-> *y* transpose to the titration curve. Print out a copy of the *net charge vs pH* curve to include with the remainder of your quiz on Wednesday.



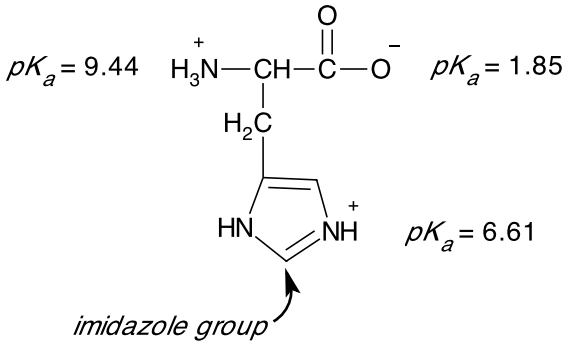

   d. At what *pH* is the protonated species shown above the most predominant? $Endpoint_2 = 7.36$

Name _____

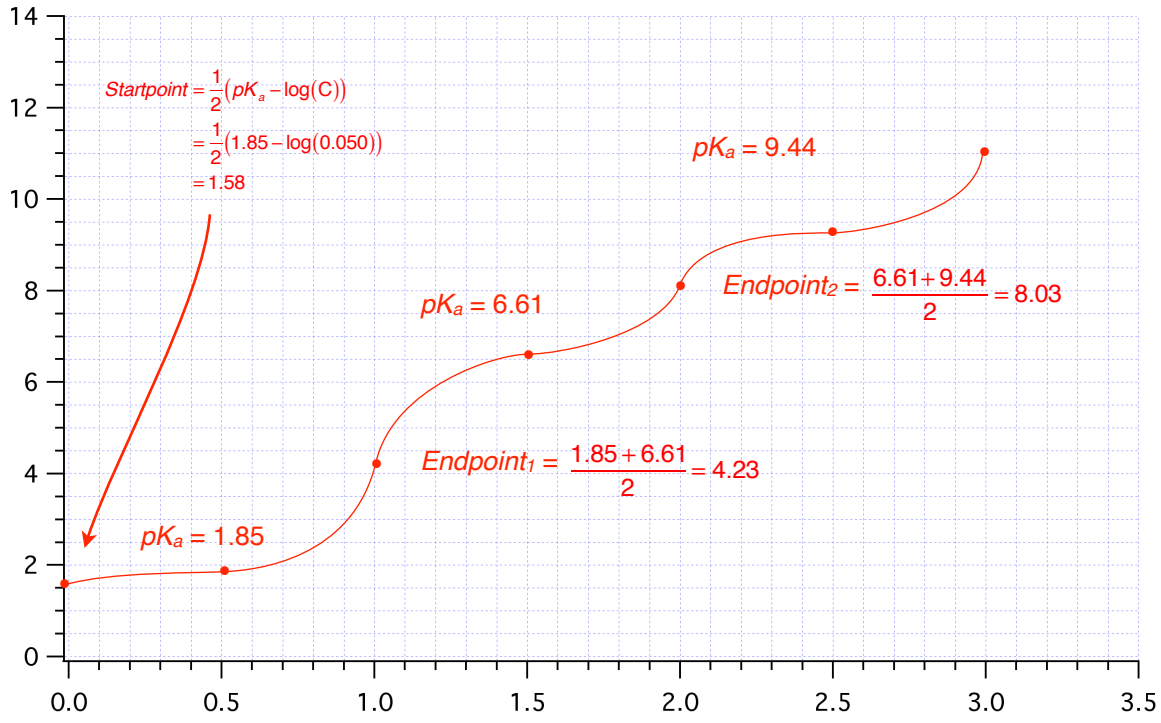
# Chem 352 - Fall 2013
# Quiz 1 (In class portion)

*R* = 8.314 *J/(mol•K)* = 0.08206 *(L•atm)/(mol•K)*

2. Histidine is one of the 20 common amino acids and has a side chain comprising an imidazole group. The structure for histidine in one of its partially protonated forms is shown below, along with the $pK_a$ values for each of its titratable groups, as determined at 25°C:



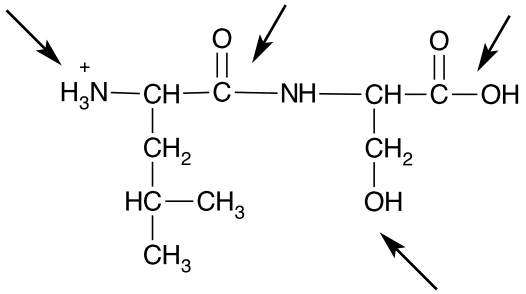

a. *Sketch the titration* curve for a 50 mM solution of histidine (Be sure to label the axes.):

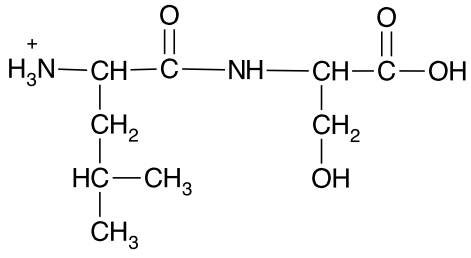



b. At what *pH* does the species shown above predominant? $Endpoint_1 = 4.23$

c. Calculate the standard free energy change ($\Delta G°'$) in kJ/mol at 25°C for the dissociation of a proton from the *imidazole side-chain group* of histidine?

3. Two structures for the dipeptide made from the amino acids leucine and serine are shown below.
   a. For the structure *at the top*, *label* each of the functional groups that are highlighted with arrows.
   b. For the structure *at the bottom*, *circle and label one example* of a portion of the molecule that can participate in each of the following non-covalent interactions:
      i. Label "A" for hydrogen bond as a donor
      ii. Label "B" for hydrophobic interaction
      iii. Label "C" for charge/charge interaction
      iv. Label "D" for dipole/dipole interaction
      v. Label "E" for hydrogen bond as an acceptor





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