1. (4 pts, 5 min) Two thin hollow tubes are held up-right in a basin of water. The first tube is made of a plastic (polyethylene) and the second tube is made of glass. The water rises in the tube made of glass, but does not in the plastic tube. Why? What is the likely difference between the surface of the plastic tube and the glass tube.

   The plastic is non-polar and has no hydrogen bond donors or acceptors, therefore the water cannot interact with it via hydrogen bonds and cannot climb up the surface. Glass must have polar surface.

2. (2 pts, 5 min) Two solutions have pH values of 7 and 10, respectively. What is their ratio of hydrogen ion (hydronium ion) concentrations? Which has the higher concentration of hydrogen ions?

   \[ \text{pH} = -\log[H^+] \]. Therefore, \[ [H^+] = 10^{-\text{pH}} \].

   \( \text{pH} = 7, \quad [H^+] = 10^{-7} \)
   \( \text{pH} = 10, \quad [H^+] = 10^{-10} \)

   Ratio of the two hydrogen ion concentrations is 1000, pH 7 has the higher concentration.

3. (4 pts, 5 min) Nitrogen typically forms three covalent bonds. Explain how nitrogen can form four bonds in the ammonium ion, \( \text{NH}_4^+ \).

   Nitrogen has 7 electrons. Two of these are in the 1st shell and the remaining five are in the second shell. The second shell contains four orbitals, three of these will have a single electron (that’s why nitrogen forms three bonds). The fourth is full, with two electrons. The full one can interact with the hydrogen ion when it gets protonated, since the bare proton has no electrons.

   - The same thing happens when water is protonated to produce the hydronium ion.

4. (5 pts, 5 min) The structure of the drug Benzedrine is shown on the right. It is absorbed more readily in the small intestine, where the pH=8, than in the stomach, where the pH=2.0. Why? [Hint. Identify the ionizable group on Benzedrine, and consider how its ionization state would differ at the different pH values?]

   There is an amino group – \( \text{NH}_2 \) on this drug. The pKa of this group is around 8.

   At pH=2 it would be fully protonated with a positive charge (\( \text{NH}_3^+ \)), so it would not pass through cell membranes in the stomach very effectively.

   At pH=8, more molecules would be deprotonated, and neutral. This would pass through the cell membranes in the intestines quite readily.

5. (12 pts, 20 min)

   i) Sketch, on the same graph, the curves for the fraction protonated versus pH for all of the ionizable groups on the amino acid aspartic acid. Your x-axis should go from pH=0 to 12. You can assume that the pKa values are 2, 4, and 9 for the mainchain carboxyl, the sidechain carboxyl and the amino group, respectively. The fraction protonated curves are plotted on the right.
ii) Draw the amino acid aspartic acid in its correct ionization state at pH=0 and at pH=7.

The forms of aspartic acid, at pH=0 and 7 are also shown below. All groups are protonated at pH=0 (fraction protonated for all groups is 1.0), at pH=7 both carboxylates are deprotonated (fraction protonated = 0.0), but the amino group is fully protonated (fraction protonated =1).

iii) Add a water molecule to your sketch at pH = 0, oriented so that it could form a hydrogen bond with the sidechain atoms of aspartic acid. Indicate the donor and acceptor groups in your diagram.

One possible water molecule is shown donating a hydrogen to the C=O. the –OH group on the sidechain could also act as a donor (O-H) and an acceptor (just the oxygen)

6. (5 pts, 10 min) Indicate possible hydrogen bond donors and acceptors on the compound on the right.

An X-H group is always a donor, when X=oxygen or nitrogen.

A Y atom (N, O, F) is usually an acceptor. The N-H is shown as both a donor and acceptor here (correctly). However, when the N is part of the peptide bond it can donate a hydrogen bond, but cannot accept.

7. (5 pts, 10 min) A short protein (peptide) consists of 5 amino acids. How many different proteins of this length are possible?

There are 20 common amino acids. So, there are 20 choices for the first residue, 20 for the second, 20 for the third, etc. # = (20)^5 = 3,200,000, a large number of potential proteins.

Jmol Problem:

8. (6 points, 10 min) Go to the Jmol page for this problem set and answer the following questions:

i) Draw the chemical structure of the compound. On the right.

ii) How would you classify this compound – polar, non-polar, or both? Justify your answer.

It is both – it has a non-polar ring and a polar hydrogen bond donor.

iii) What amino acid has this functional group as part of its structure?

Tryptophan

Important points/skill you should master from this problem set:

- pH scale – the lower the pH, the higher the [H+] concentration.
- The structure of protonated water (H₃O⁺), or the hydronium ion
- How pH affects whether a group is charged or not. At low pH the group becomes protonated which may either remove its charge (e.g. carboxylate, COOH) or generate a charge (e.g. amino, -NH₃⁺)
- How the presence of charges on a molecule affect its ability to cross the membrane.
- How to draw and use the fraction protonated curve to predict how much of a group is protonated
- How to identify hydrogen bond donors (O-H, N-H) and acceptors (O, N). (Don't forget that the N in the peptide bond cannot accept a hydrogen bond).
- How to determine whether a functional group is polar or non-polar and realize that a group may have both properties.