Chemistry 3785 – Problem Set # 1

Predicting Peptide Structures and Charges as a Function of pH

For each of the following peptides, draw their **Lewis** structures at the indicated pH values and calculate the net charge on the peptide.[1,2]

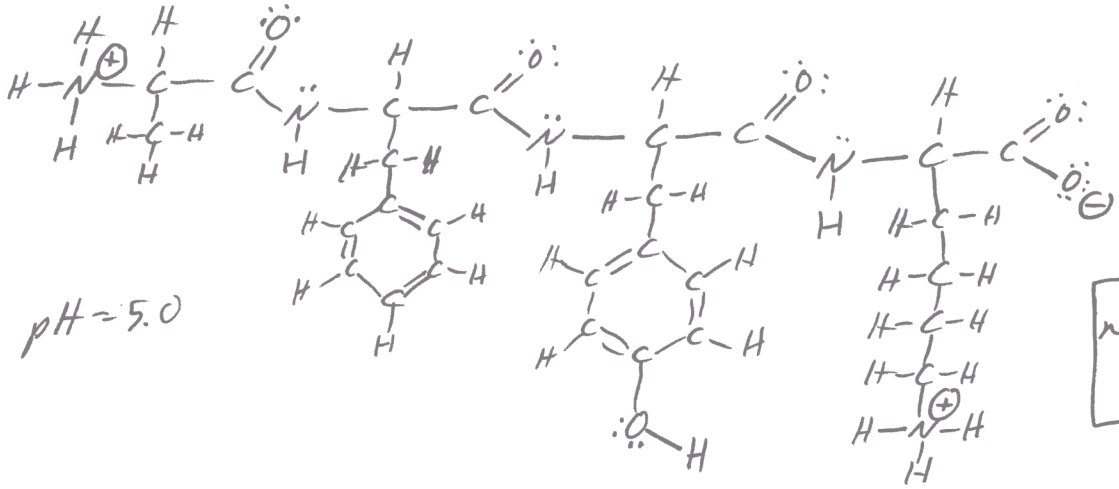
1. Ala-Phe-Tyr-Lys pH = 5.0
2. Cys-His-Arg pH = 9.5
3. Glu-Asn-Thr-Trp pH = 2.0
4. Tyr-His-Asp-Arg-His pH = 9.1
5. Pro-Hyp-Gly-Cys-Ser pH = 10.3
6. Ile-Pro-Lys-Gly-Asp pH = 6.4

[1] Note: Not for 3785 this year, but appropriate for MCAT, DCAT, GRE, etc., related studying: For each peptide, predict its isoelectric point, pI (i.e., this is the pH value at which it would have a net charge of 0) and draw its structure at this pH.

[2] Note: Hyp = Hydroxyproline

1st Problem Set

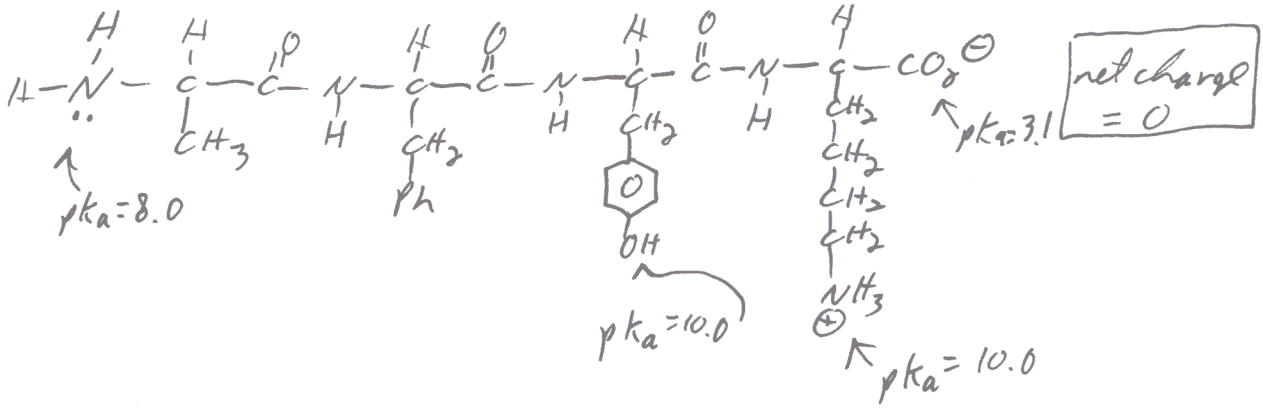
1.



pH = 5.0

net charge = +1

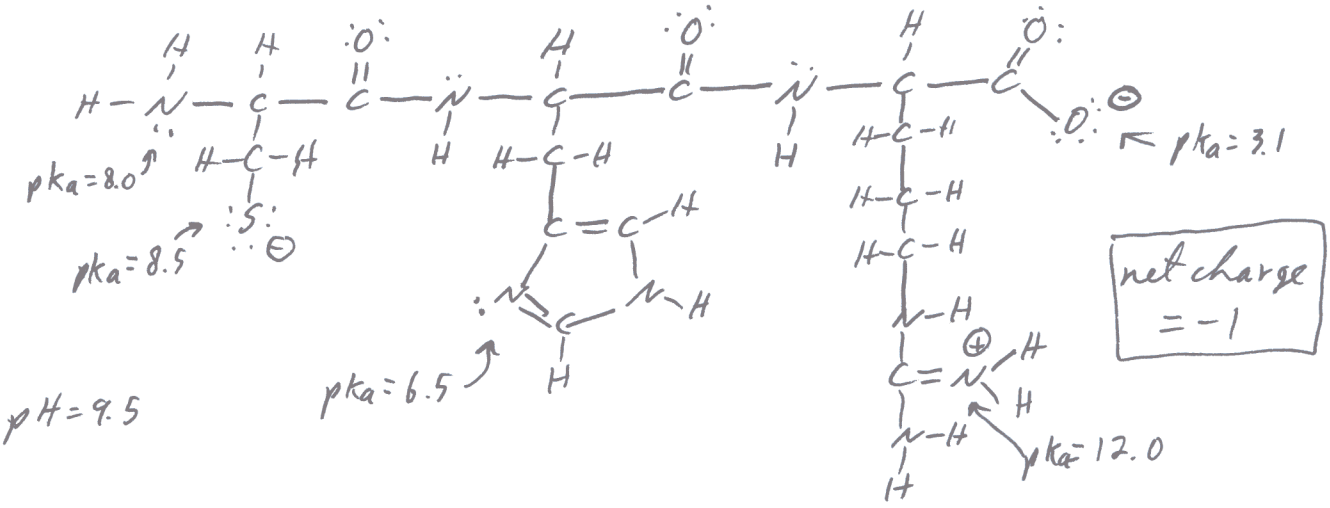
pI = 9.0 (ie the point at which the terminal amino group is deprotonated but the Lys is not yet)



net charge = 0

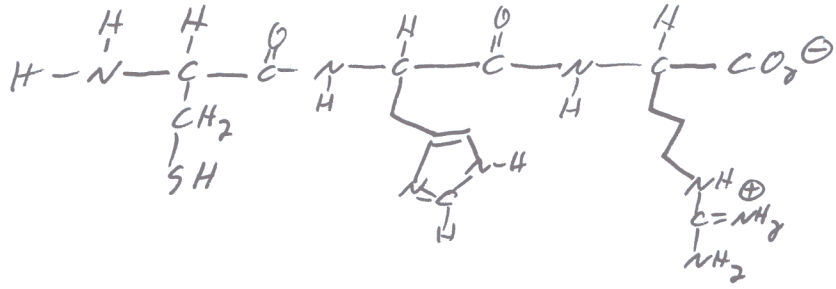
[Note: the top structure is drawn as a Lewis structure while the bottom one is not]

2.



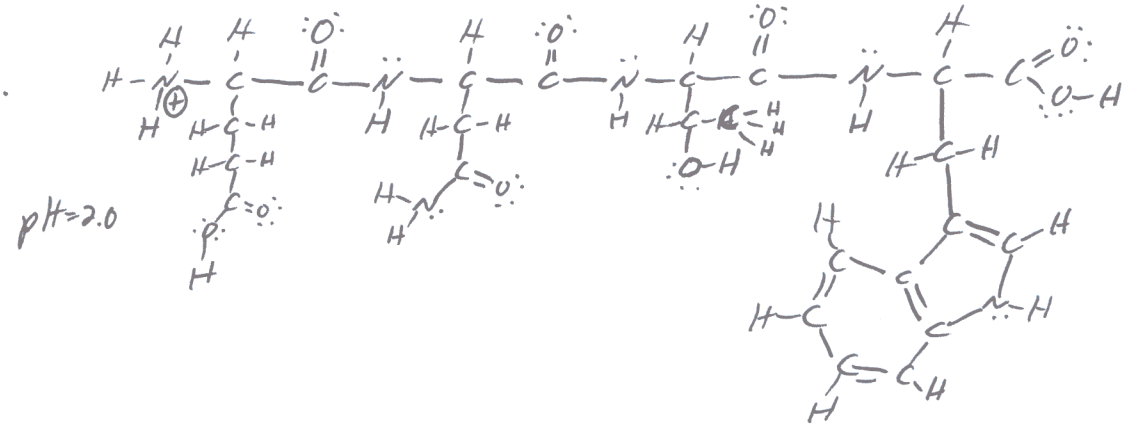
net charge = −1

pI ≈ 8.3



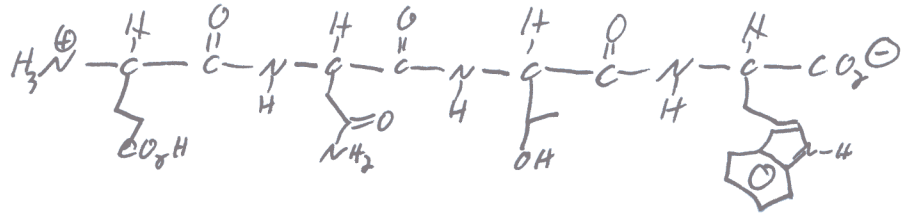
net charge = 0

3.



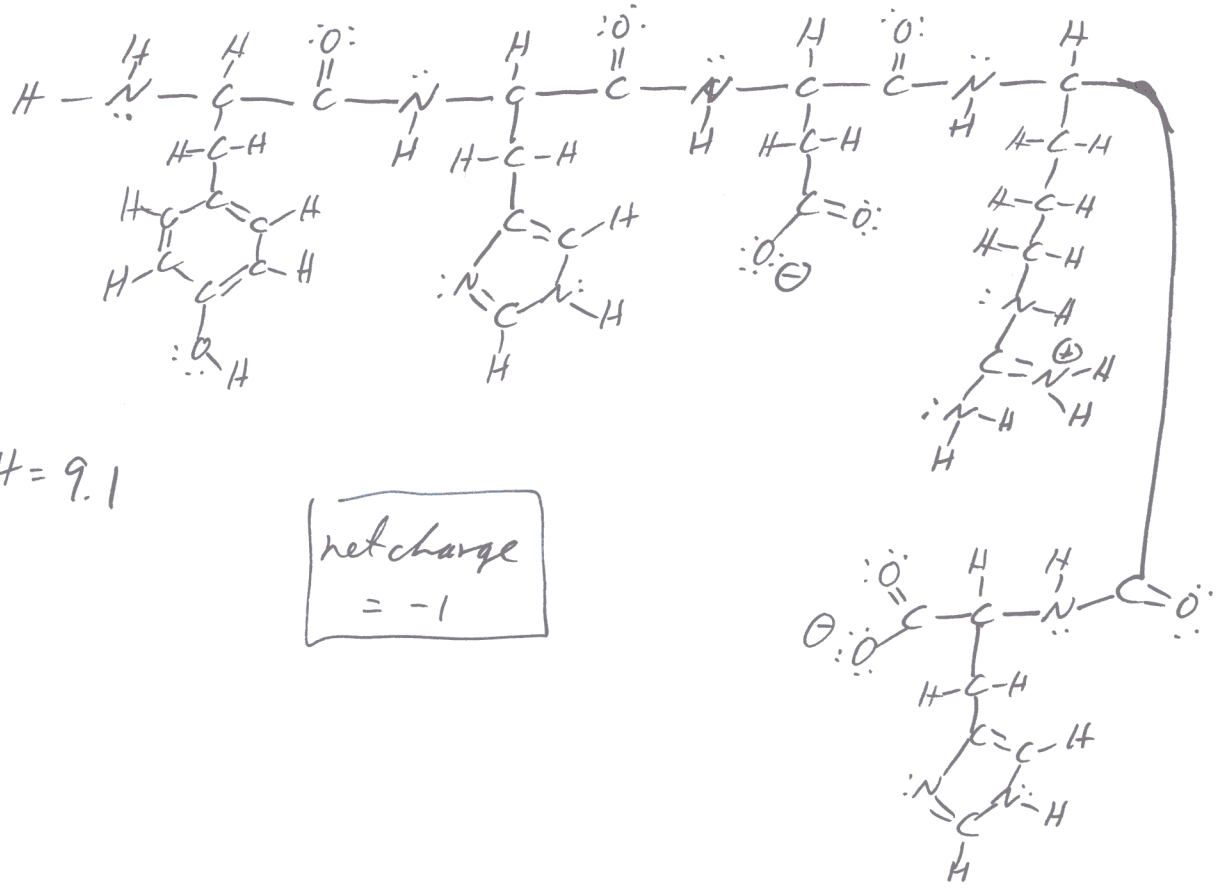
net charge = +1

pI ≈ 3.6



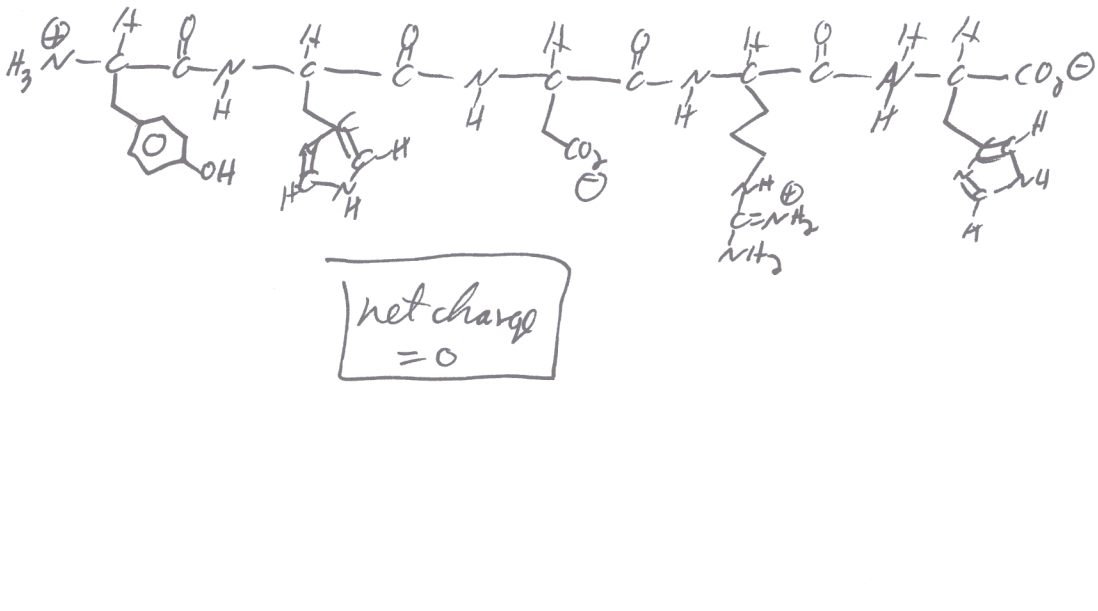
net charge = 0

4.



pH = 9.1

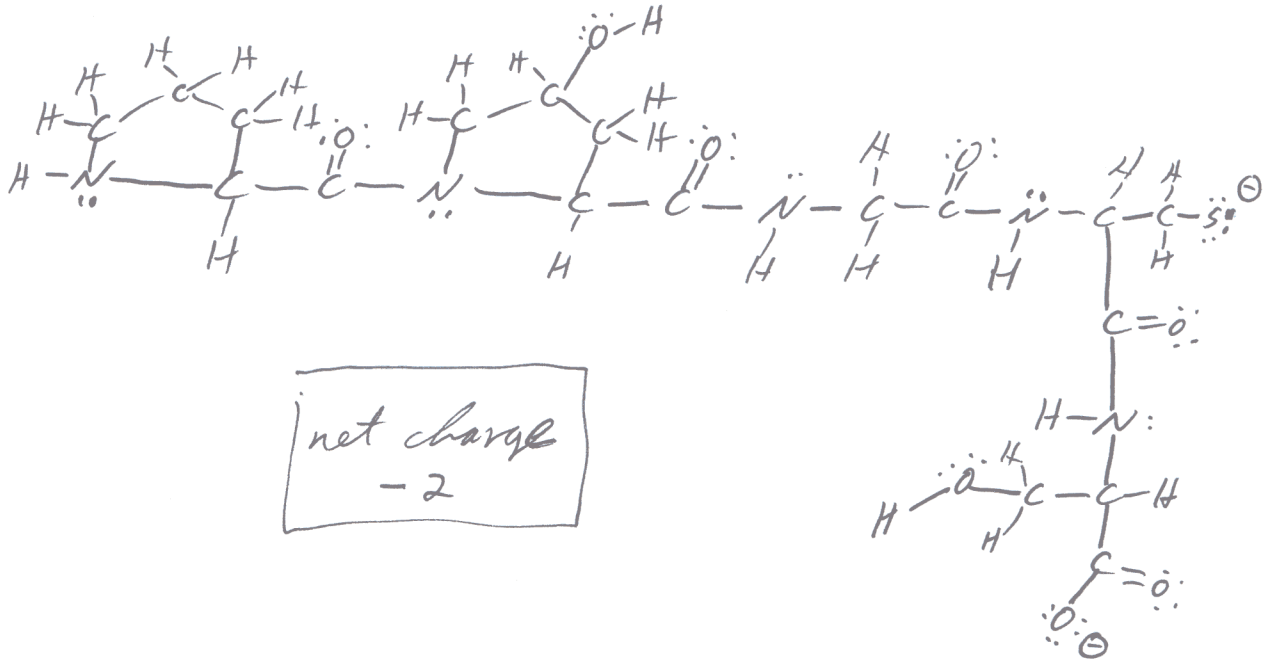
net charge = −1



pI = 7.3

net charge = 0

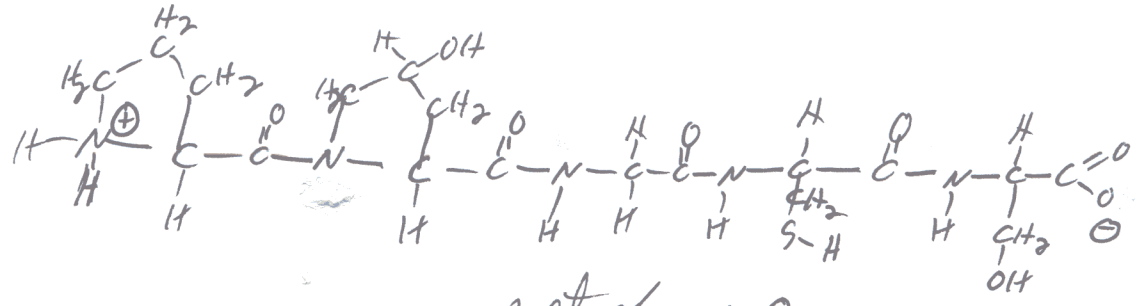
5.



pH = 10.3

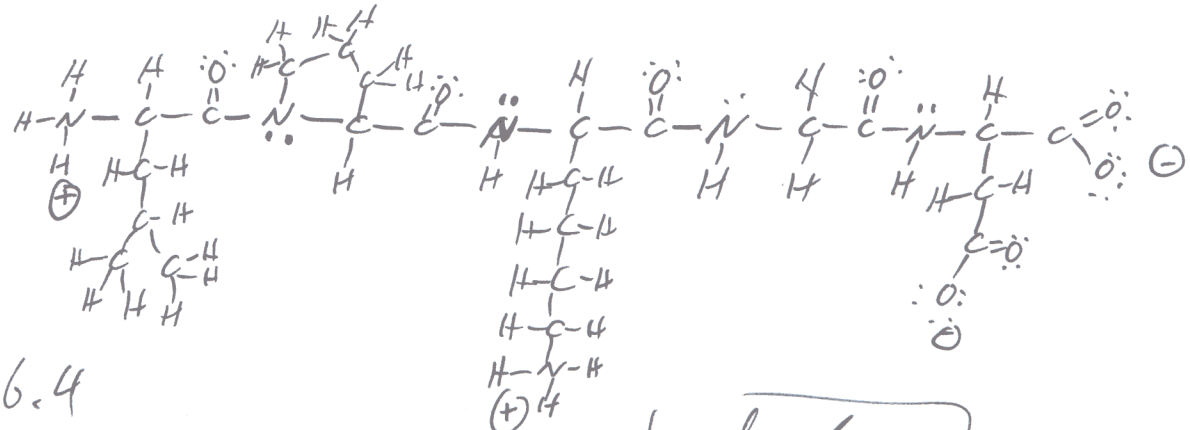
net charge
−2

pI ≈ 6



net charg = 0

6.



pH = 6.4

net charge
= 0

this is at the isoelectric point (pI = 6.4)