

Notes 10/3

Wednesday, October 03, 2007

10:00 AM

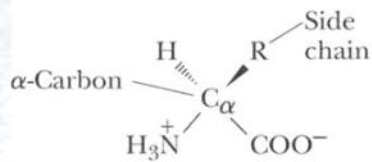
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Amino Acids: Acid-Base Properties

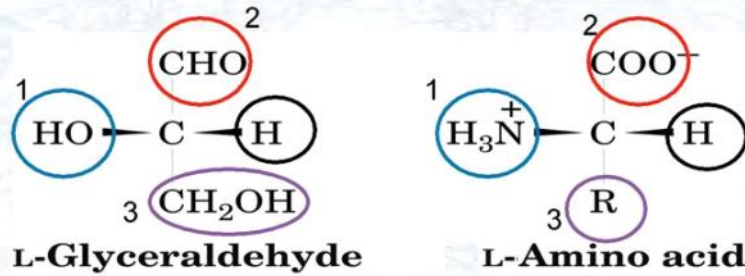
Oct. 3, 2007

Review

- Amino acids:
 - tetrahedral α carbon
 - amino group
 - carboxyl group
 - side chain (R group)
- Peptide bonds
- Classification: nonpolar, polar, acidic, basic



L-amino acid configuration is based on L-glyceraldehyde's configuration



Priorities

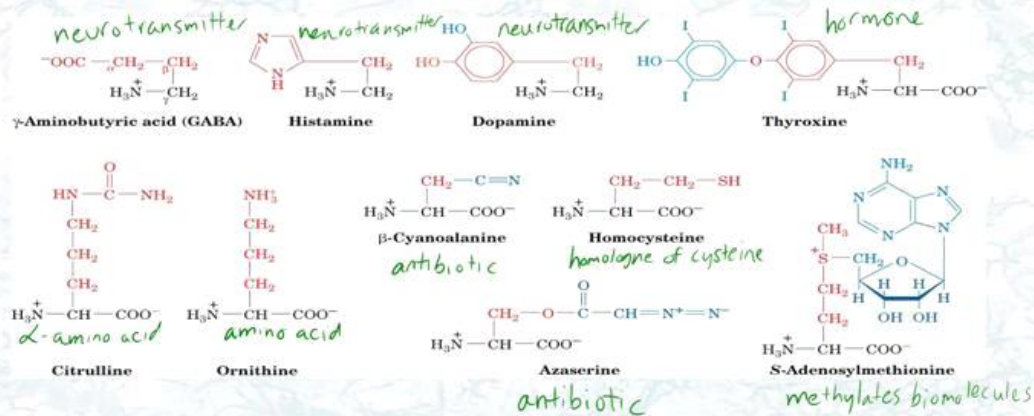
$\text{SH} > \text{OH} > \text{NH}_2 > \text{CH}_2\text{SH} > \text{COOH} > \text{CHO} > \text{CH}_2\text{OH} > \text{C}_6\text{H}_5$

$> \text{C}_6\text{H}_5 > \text{C}_6\text{H}_{11} > \text{CH}_3 > \text{H}$

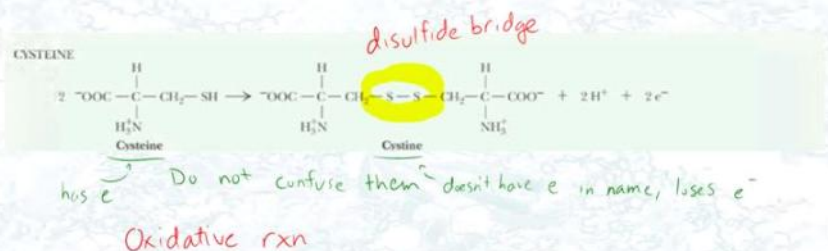
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Some biologically produced derivatives of "standard" amino acids and amino acids that are not components of proteins.

should be able to recognize structures - give name and significance

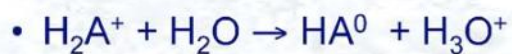


Structure of cystine

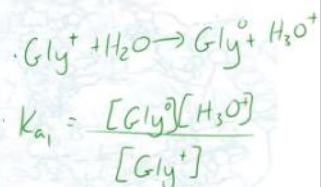


What Are Acid-Base Properties of Amino Acids?

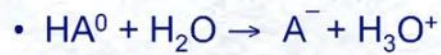
- Amino Acids are Weak Polyprotic Acids



- $$K_{a1} = \frac{[\text{HA}^0][\text{H}_3\text{O}^+]}{[\text{H}_2\text{A}^+]}$$



The second dissociation (the amino group in the case of glycine):

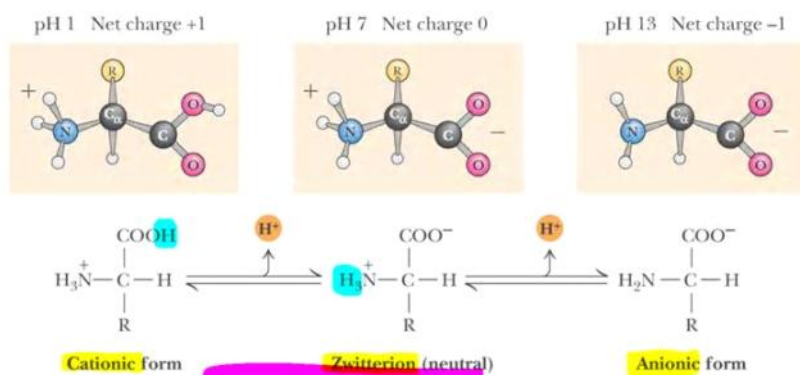


- $K_{a2} = \frac{[\text{A}^-][\text{H}_3\text{O}^+]}{[\text{HA}^0]}$



- $K_{a2} = \frac{[\text{Gly}^-][\text{H}_3\text{O}^+]}{[\text{Gly}^0]}$

The ionic forms of the amino acids, shown without consideration of any ionizations on the side chain



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pK_a of $\alpha\text{-COOH} \rightarrow 2$
 pK_a of $\alpha\text{-NH}_3 \rightarrow 9$

~ values approximate but show why COOH loses H^+ first

pK_a Values of the Amino Acids and their ionizable R-groups

Depend on T , ionic strength, and microenvironment of ionizable group

You should know these numbers and know what they mean!

- Alpha carboxyl group - $pK_a = 2$
- Alpha amino group - $pK_a = 9$
- These numbers are approximate, but entirely suitable for our purposes.

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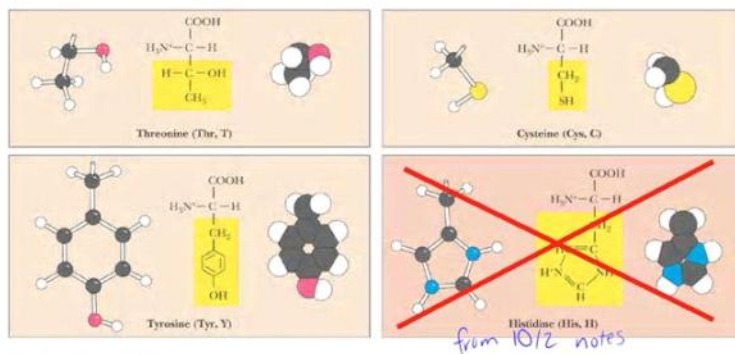
Covalent Structures and Abbreviations of the "Standard" Amino Acids of Proteins and the pK Values of Their Ionizable Groups.

Name, Three-letter Symbol, and One-letter Symbol	Structural Formula ^a	pK_a $\alpha\text{-NH}_3^+$ ^d	pK_a Side Chain ^e
Amino acids with nonpolar side chains			
Glycine Gly G	<chem>NC(=O)O</chem>	9.78	
Alanine Ala A	<chem>CC(N)C(=O)O</chem>	9.87	
Valine Val V	<chem>CC(C)C(N)C(=O)O</chem>	9.74	
Isoleucine Ile I	<chem>CC(C)C(C)C(N)C(=O)O</chem>	9.74	
Proline Pro P	<chem>C1CCN(C1)C(=O)O</chem>	10.64	
Phenylalanine Phe F	<chem>c1ccc(cc1)C(C(N)C(=O)O)C(=O)O</chem>	9.31	
Tryptophan Trp W	<chem>c1ccc2c(c1)c(c[nH]2)C(C(N)C(=O)O)C(=O)O</chem>	9.41	
Amino acids with charged polar side chains			
Serine Ser S	<chem>CC(O)C(N)C(=O)O</chem>	2.19	9.21
Threonine Thr T	<chem>CC(C)C(O)C(N)C(=O)O</chem>	2.09	9.10
Asparagine ^c Asn N	<chem>CC(N)C(=O)N</chem>	2.14	8.72
Glutamine ^c Gln Q	<chem>CCC(N)C(=O)N</chem>	2.17	9.13
Tyrosine Tyr Y	<chem>c1ccc(cc1)C(C(N)C(=O)O)C(=O)O</chem>	2.20	9.21
Cysteine Cys C	<chem>CC(S)C(N)C(=O)O</chem>	1.92	10.70
Amino acids with charged polar side chains			
Lysine Lys K	<chem>CCCC[NH3+]</chem>	2.18	9.06
Arginine ^c Arg R	<chem>CCC[NH3+]</chem>	1.82	8.99
Histidine ^c His H	<chem>c1ccc(cc1)[nH]c1cc[nH]c1</chem>	1.80	9.33
Aspartic acid ^c Asp D	<chem>CC(=O)[O-]</chem>	1.99	9.80
Glutamic acid ^c Glu E	<chem>CCC(=O)[O-]</chem>	2.10	9.47

(continued)

10.5 (pKa)
8.4 (pKa) ← know these
10.5 (pKa)
12.5 (pKa)
10 (pKa)
3.9 (pKa)
4.4 (pKa)

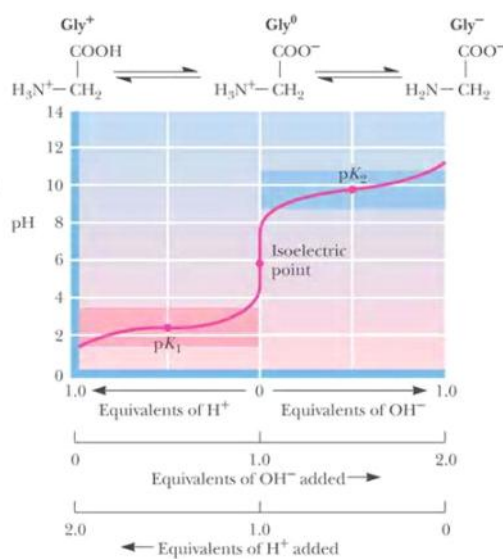
Polar, neutral



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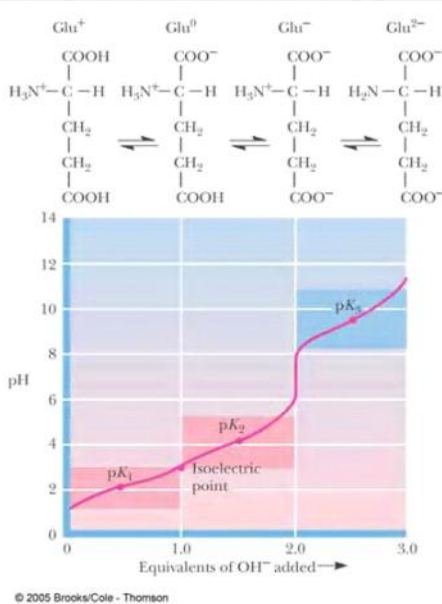
Garrett and Grisham, Biochemistry, Third Edition

Titration of glycine, a simple amino acid.



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Titration of glutamic acid.



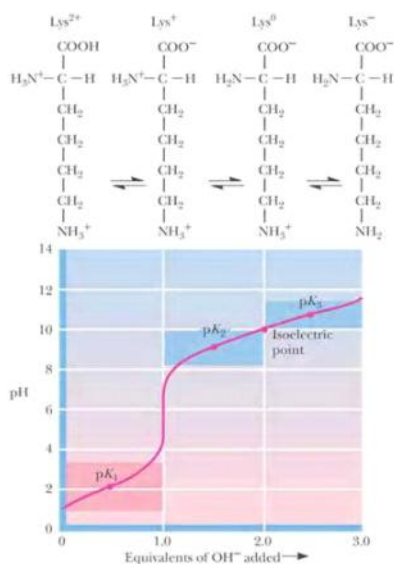
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A Sample Calculation

What is the pH of a glutamic acid solution if the alpha carboxyl is 1/4 dissociated?

- $\text{pH} = 2 + \log \frac{[1]}{[3]}$
- $\text{pH} = 2 + (-0.477)$
- $\text{pH} = \underline{1.5}$

Titration of lysine.



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Another Sample Calculation

What is the pH of a lysine solution if the side chain amino group is 3/4 dissociated?

- $\text{pH} = 10.5 + \log \frac{[3]}{[1]}$ $\frac{A^-}{HA}$
- $\text{pH} = 10.5 + (0.477)$
- $\text{pH} = \underline{10.977 \approx 11}$