

## Notes 10/3

Wednesday, October 03, 2007  
10:00 AM

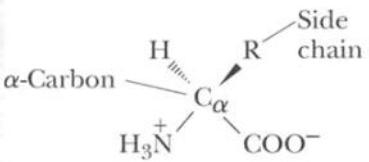
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## Amino Acids: Acid-Base Properties

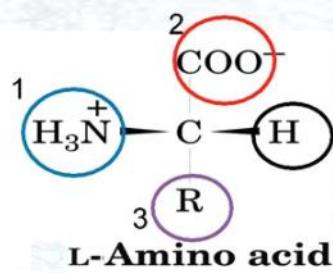
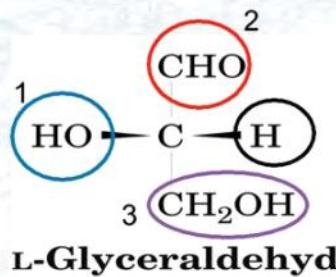
Oct. 3, 2007

## Review

- Amino acids:
  - tetrahedral  $\alpha$  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



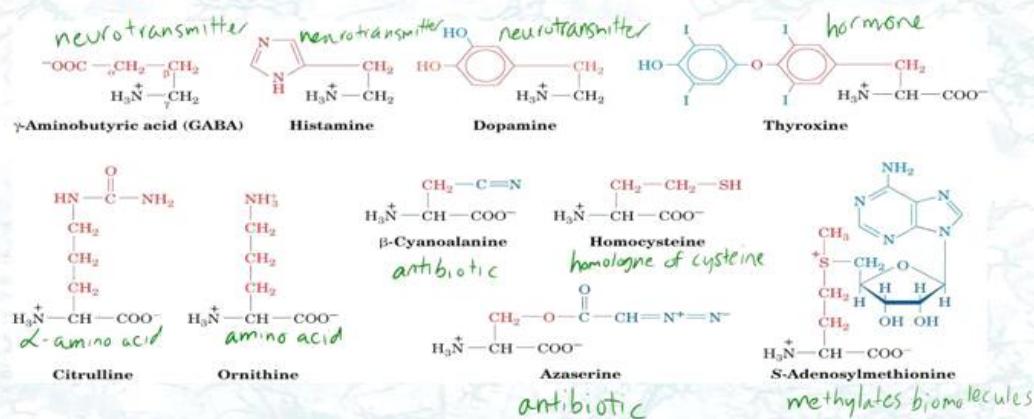
Priorities

SH > OH > NH<sub>2</sub> > CH<sub>2</sub>SH > COOH > CHO > CH<sub>2</sub>OH > C<sub>6</sub>H<sub>5</sub>  
> C<sub>6</sub>H<sub>5</sub> > C<sub>6</sub>H<sub>11</sub> > CH<sub>3</sub> > H

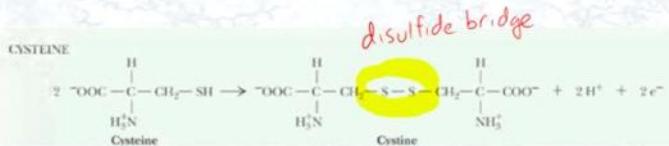
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Some biologically produced derivatives of "standard" amino acids and amino acids that are not components of proteins.

Should be able to recognize structures - give name and significance



## Structure of cystine

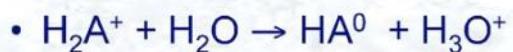


hus e Do not confuse them doesn't have e in name, loses e-

## Oxidative rxn

## What Are Acid-Base Properties of Amino Acids?

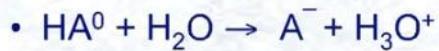
- Amino Acids are Weak Polyprotic Acids



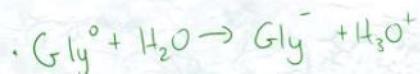
$$\bullet K_{a1} = \frac{[ HA^0 ] [ H_3O^+ ]}{[ H_2A^+ ]}$$

$$K_{a_1} = \frac{[Gly^0][H_3O^+]}{[Gly^+]}$$

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



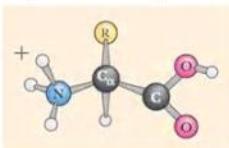
$$\cdot K_{a2} = \frac{[\text{A}^-][\text{H}_3\text{O}^+]}{[\text{HA}^0]}$$



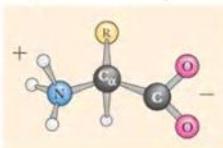
$$\cdot K_{a2} = \frac{[\text{Gly}^-][\text{H}_3\text{O}^+]}{[\text{Gly}^0]}$$

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

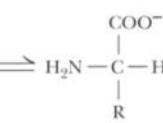
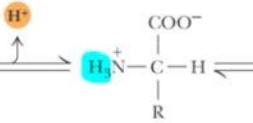
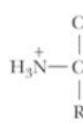
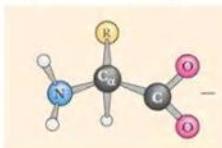
pH 1 Net charge +1



pH 7 Net charge 0



pH 13 Net charge -1



Cationic form

Zwitterion (neutral)

Anionic form

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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  $\text{COOH}$  loses  $\text{H}^+$  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!

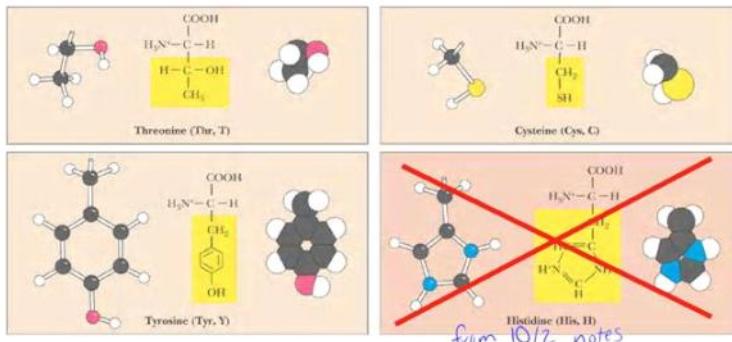
- Alpha carboxyl group -  $pK_a = 2$
- Alpha amino group -  $pK_a = 9$
- These numbers are approximate, but entirely suitable for our purposes.

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

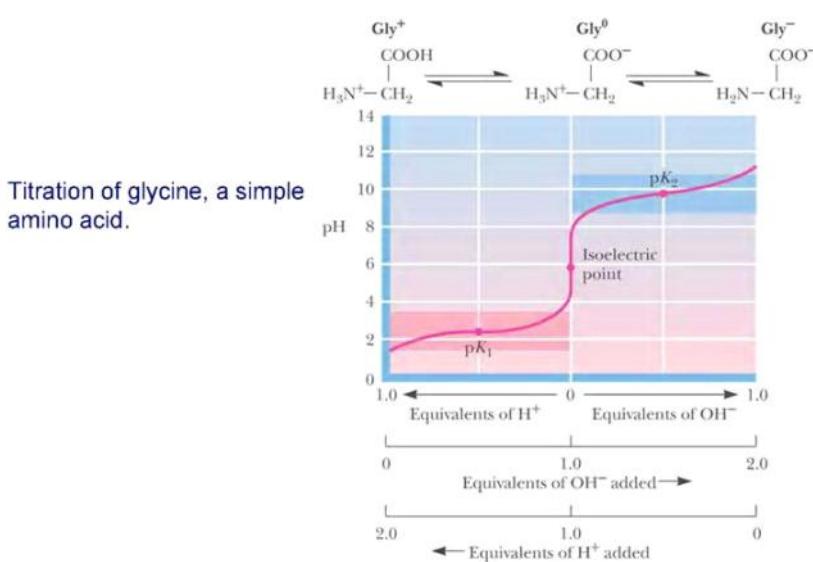
Name, Three-letter Symbol, and One-letter Symbol	Structural Formula <sup>a</sup>	$pK_a$ $\alpha\text{-NH}_3^+$ <sup>b</sup>	$pK_a$ Side Chain <sup>b</sup>	Name Three-letter Symbol, and One-letter Symbol	Structural Formula <sup>a</sup>	$pK_a$ $\text{COOH}^+$ <sup>b</sup>	$pK_a$ $\text{NH}_3^+$ <sup>b</sup>	$pK_a$ Side Chain <sup>b</sup>					
<b>Amino acids with nonpolar side chains</b>													
Glycine Gly	<chem>CC</chem>	9.78		Serine Ser	<chem>CC(O)N</chem>	2.19	9.21						
Alanine Ala	<chem>CC(N)C</chem>	9.87		Threonine Thr	<chem>CC(O)C(O)N</chem>	2.09	9.10						
Valine Val	<chem>CC(C)N</chem>	9.74		Asparagine <sup>c</sup> Asn	<chem>CC(O)C(=O)N</chem>	2.34	8.72						
Leucine Leu	<chem>CC(C)C(N)C</chem>	9.74		Glutamine <sup>c</sup> Gln	<chem>CC(O)C(=O)NCC</chem>	2.17	9.13						
Isoleucine Ile	<chem>CC(C)C(C)N</chem>	9.76		Tyrosine Tyr	<chem>CC(O)C(=O)c1ccc(O)cc1</chem>	2.20	9.21						
Methionine Met	<chem>CC(C)CS(=O)(=O)N</chem>	9.28		Cysteine Cys	<chem>CC(O)C(=O)SC</chem>	1.92	10.76						
Proline Pro	<chem>C1CC(C)N1</chem>	10.64		<i>10.57 fine</i> <i>know these</i>									
Phenylalanine Phe	<chem>CC(C)C1=CC=CC=C1</chem>	9.31		<i>8.4 fine</i> <i>know these</i>									
Tryptophan Trp	<chem>CC(C)C1=CC2=C(C=C1)N=C2</chem>	9.41		<i>10.6 NH</i>									
<i>(continued)</i>													
<b>Amino acids with uncharged polar side chains</b>													
Lysine Lys	<chem>CC(C)C(N)N</chem>	2.16	9.66	Lysine Lys	<chem>CC(C)C(N)N</chem>	2.16	9.66						
Arginine Arg	<chem>CC(C)C(N)C(=O)N</chem>	1.82	9.89	Arginine Arg	<chem>CC(C)C(N)C(=O)N</chem>	1.82	9.89	<i>12.5 (imidazole)</i>					
Histidine His	<chem>CC(C)C1=CSC=C1</chem>	1.80	9.53	Histidine His	<chem>CC(C)C1=CSC=C1</chem>	1.80	9.53	<i>6.0 (imidazole)</i>					
Aspartic acid Asp	<chem>CC(O)C(=O)O</chem>	1.99	9.90	Aspartic acid Asp	<chem>CC(O)C(=O)O</chem>	1.99	9.90	<i>3.9 COOH</i>					
Glutamic acid Glu	<chem>CC(O)C(=O)O</chem>	2.30	9.47	Glutamic acid Glu	<chem>CC(O)C(=O)O</chem>	2.30	9.47	<i>4.7 COOH</i>					

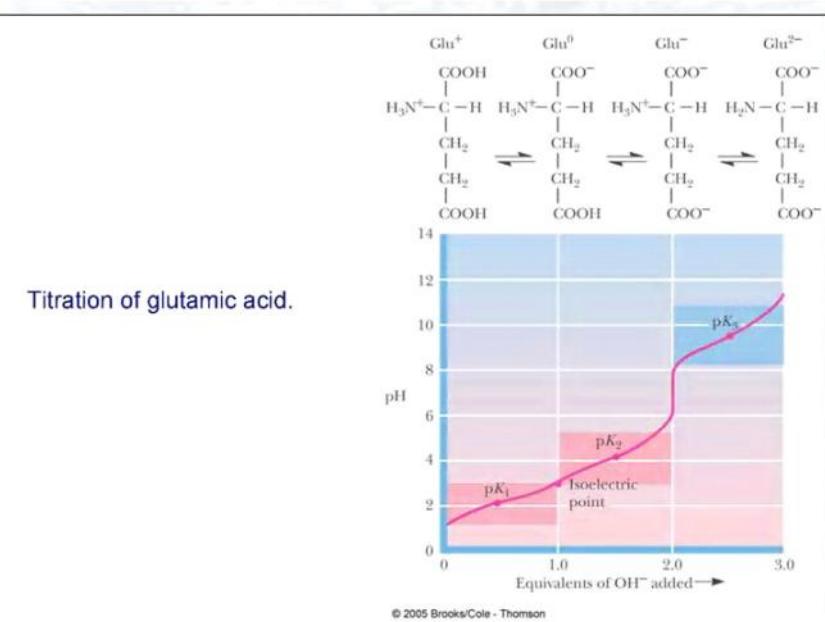
## Polar, neutral



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Carroll and Graham, Biochemistry, Third Edition





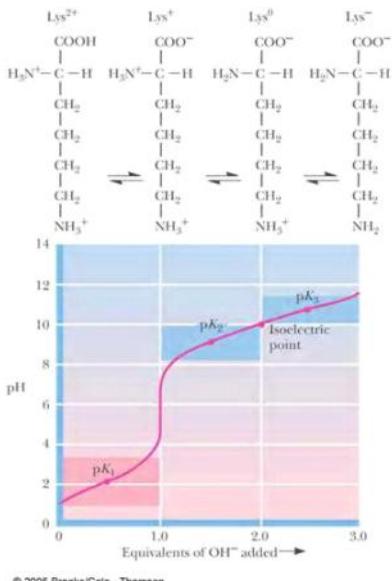
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## A Sample Calculation

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

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

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?

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