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# CEE 370 Environmental Engineering Principles

## Lecture #8 Environmental Chemistry VI: Acids- bases III, Organic Nomenclature

**Reading:** Mihelcic & Zimmerman, Chapter 3

Davis & Masten, Chapter 2  
Mihelcic, Chapt 3

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## Steps in Solving chemical equilibria

1. List all chemical species or elemental groupings that are likely to exist
  - Cations:  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{+2}$ ,  $\text{NH}_4^+$ ,  $\text{H}^+$ , etc.
  - Anions:  $\text{NO}_3^-$ ,  $\text{Cl}^-$ ,  $\text{SO}_4^{-2}$ ,  $\text{OH}^-$ ,  $\text{PO}_4^{-3}$ ,  $\text{HPO}_4^{-2}$ ,  $\text{H}_2\text{PO}_4^-$ ,  $\text{Ac}^-$ ,  $\text{HCO}_3^-$ ,  $\text{CO}_3^{-2}$ , etc.
  - Neutral species:  $\text{NH}_3$ ,  $\text{HAc}$ ,  $\text{H}_3\text{PO}_4$ ,  $\text{H}_2\text{CO}_3$ , etc.
  - note that ionic salts (e.g.,  $\text{NaCl}$ ,  $\text{KCl}$ ) completely dissociate in water and thus should not be listed.

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Showing an example of  $10^{-3}$   $\text{NaCO}_3$  added to water

## Steps in Solving chemical equilibria (cont)

2. List all independent chemical equations that involve the species present, including:

A. Chemical Equilibria

- E.g., acid base equilibria

$$K_1 = \frac{[H^+][HCO_3^-]}{[H_2CO_3]} = 10^{-6.3}$$

$$K_2 = \frac{[H^+][CO_3^{2-}]}{[HCO_3^-]} = 10^{-10.3}$$

B. Mass Balance equations

- Total amount of each element is conserved

$$C_{\text{carbonates}} = [H_2CO_3] + [HCO_3^-] + [CO_3^{2-}] = 10^{-3} \quad \text{and} \quad C_{\text{sodium}} = [Na^+] = 10^{-3}$$

C. Electroneutrality or charge balance

- All water solutions must be neutrally charged

$$[H^+] + [Na^+] = [OH^-] + [HCO_3^-] + 2[CO_3^{2-}]$$

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## Steps in Solving chemical equilibria (cont)


3. Solve the equations

- You should have as many independent equations as chemical species
- Often it is easiest to solve for  $H^+$  and then use that concentration to calculate all other species

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## Example 4.11

Determine the species present if the following compounds are dissolved into water, in both open and closed systems:

- Sodium carbonate,  $[\text{Na}_2\text{CO}_3]$
- Sodium bicarbonate,  $[\text{NaHCO}_3]$
- Sodium phosphate,  $[\text{Na}_3\text{PO}_4]$

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## Solution to 4.11 a)

First the sodium carbonate will dissolve

$$\text{Na}_2\text{CO}_3(\text{s}) \rightarrow 2\text{Na}^{2+} + \text{CO}_3^{2-}$$

Then the carbonate can become protonated

$$\text{H}^+ + \text{CO}_3^{2-} \leftrightarrow \text{HCO}_3^-$$


$$\text{H}^+ + \text{HCO}_3^- \leftrightarrow \text{H}_2\text{CO}_3(\text{aq})$$

$$\text{H}_2\text{CO}_3(\text{aq}) \leftrightarrow \text{H}_2\text{O} + \text{CO}_2(\text{aq})$$

Finally, in an open system, the carbon dioxide can escape as a gas

$$\text{CO}_2(\text{aq}) \leftrightarrow \text{CO}_2(\text{g})$$

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## Solution to 4.11 b)

First the sodium bicarbonate will dissolve

$$\text{NaHCO}_3(\text{s}) \rightarrow \text{Na}^+ + \text{HCO}_3^-$$

Then the bicarbonate can become protonated or deprotonated

$$\text{H}^+ + \text{CO}_3^{2-} \leftrightarrow \text{HCO}_3^-$$


$$\text{H}^+ + \text{HCO}_3^- \leftrightarrow \text{H}_2\text{CO}_3(\text{aq})$$

$$\text{H}_2\text{CO}_3(\text{aq}) \leftrightarrow \text{H}_2\text{O} + \text{CO}_2(\text{aq})$$

Finally, in an open system, the carbon dioxide can escape as a gas

$$\text{CO}_2(\text{aq}) \leftrightarrow \text{CO}_2(\text{g})$$

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## Solution to 4.11 c)

First the sodium phosphate will dissolve

$$\text{Na}_3\text{PO}_4 \rightarrow 3\text{Na}^+ + \text{PO}_4^{3-}$$

Then the phosphate can become protonated


$$\text{H}^+ + \text{PO}_4^{3-} \leftrightarrow \text{HPO}_4^{2-}$$

$$\text{H}^+ + \text{HPO}_4^{2-} \leftrightarrow \text{H}_2\text{PO}_4^-$$

$$\text{H}^+ + \text{H}_2\text{PO}_4^- \leftrightarrow \text{H}_3\text{PO}_4(\text{aq})$$

Finally, in an open system, there are no additional species to consider, because there are no gas-phase forms of phosphate

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## Carbon Forms: Definitions


**Inorganic Carbon (+IV oxidation state)**

$\text{CO}_2$  = carbon dioxide (dissolved and gas)  
 $\text{H}_2\text{CO}_3$  = carbonic acid (dissolved)  
 $\text{HCO}_3^-$  = bicarbonate (dissolved)  
 $\text{CO}_3^{-2}$  = carbonate (dissolved)  
 $\text{CaCO}_3$  = calcium carbonate (mineral)

**Organic Carbon (< +IV oxidation state)**

$\text{C}_6\text{H}_{12}\text{O}_6$  = glucose (a sugar)  
 $\text{CH}_3\text{COOH}$  = acetic acid (a carboxylic acid)

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## The Carbonate System

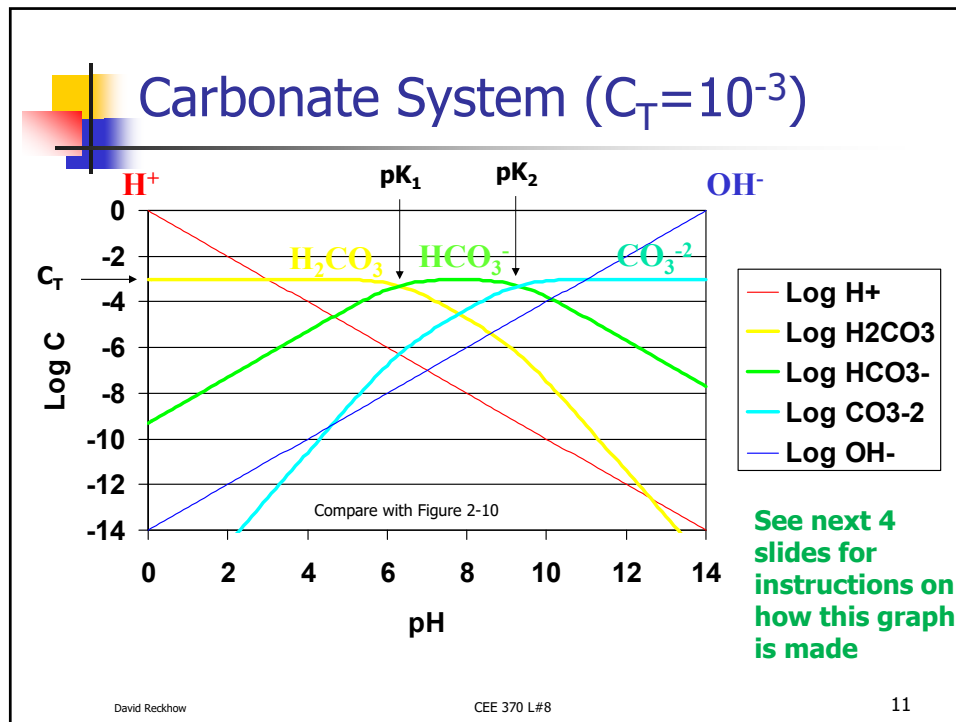
$$\text{CO}_2(\text{aq}) + \text{H}_2\text{O} \leftrightarrow \text{H}_2\text{CO}_3$$

- Major buffer ions
- volatile: interaction with atmosphere
- biologically active
- Definitions:

$$[\text{CO}_2(\text{aq})] + [\text{H}_2\text{CO}_3] = [\text{H}_2\text{CO}_3^*]$$

$$[\text{H}_2\text{CO}_3^*] + [\text{HCO}_3^-] + [\text{CO}_3^{-2}] = C_T$$

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### Rapid Method for Log C vs. pH Graph

1. Plot diagonal  $[H^+]$  and  $[OH^-]$  lines
2. Draw a light horizontal line corresponding to  $\log C_T$
3. Locate System Point
  - i.e.,  $pH = pK_a$ ,  $\log C = \log C_T$
  - make a mark 0.3 units below system point
4. Draw  $45^\circ$  lines (slope =  $\pm 1$ ) below  $\log C_T$  line, and aimed at system point
5. Approximate curved sections of species lines  $\pm 1$  pH unit around system point
6. Repeat steps as necessary for more complex graphs
  - #3-#5 for additional  $pK_a$ s of polyprotic acids
  - #2-#5 for other acid/base pairs

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## Diprotic acids: calculations

- Start with  $C_T$  and  $K_a$  equations

$$K_1 = \frac{[H^+][HA^-]}{[H_2A]}$$

$$[HA^-] = \frac{K_1[H_2A]}{[H^+]}$$

$$C_T = [H_2A] + [HA^-] + [A^{-2}]$$

$$K_2 = \frac{[H^+][A^{-2}]}{[HA^-]}$$

$$[A^{-2}] = \frac{K_2[HA^-]}{[H^+]}$$

$$= \frac{K_1 K_2 [H_2A]}{[H^+]^2}$$

$$C_T = [H_2A] + \frac{K_1[H_2A]}{[H^+]} + \frac{K_1 K_2 [H_2A]}{[H^+]^2}$$

$$C_T = [H_2A] \left( 1 + \frac{K_1}{[H^+]} + \frac{K_1 K_2}{[H^+]^2} \right)$$

$$\frac{[H_2A]}{C_T} = \frac{1}{1 + \frac{K_1}{[H^+]} + \frac{K_1 K_2}{[H^+]^2}}$$

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## Diprotic acids: calculations (cont.)

- Use  $[H_2A]/C_T$  and  $K_a$  equations to get other  $\alpha$ 's

$$K_1 = \frac{[H^+][HA^-]}{[H_2A]} \rightarrow \frac{K_1}{[H^+]} = \frac{[HA^-]}{[H_2A]}$$

$$K_2 = \frac{[H^+][A^{-2}]}{[HA^-]} \rightarrow \frac{K_2}{[H^+]} = \frac{[A^{-2}]}{[HA^-]}$$

For distribution diagrams

$$\frac{[H_2A]}{C_T} = \frac{1}{1 + \frac{K_1}{[H^+]} + \frac{K_1 K_2}{[H^+]^2}}$$

**$\alpha_0$**

$$\frac{[HA^-]}{C_T} = \frac{1}{\frac{[H^+]}{K_1} + 1 + \frac{K_2}{[H^+]}}$$

**$\alpha_1$**

$$\frac{[A^{-2}]}{C_T} = \frac{1}{\frac{[H^+]^2}{K_1 K_2} + \frac{[H^+]}{K_2} + 1}$$

**$\alpha_2$**

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CEE 370 L#8 Note:  $\alpha_0 + \alpha_1 + \alpha_2 = 1$ 
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## Diprotic acids: calculations (cont.)

$\alpha_0 \equiv \frac{[H_2A]}{C_T}$ $\frac{1}{1 + \frac{K_1}{[H^+]} + \frac{K_1K_2}{[H^+]^2}}$	$\alpha_1 \equiv \frac{[HA^-]}{C_T}$ $\frac{1}{\frac{[H^+]}{K_1} + 1 + \frac{K_2}{[H^+]}}$	$\alpha_2 \equiv \frac{[A^{2-}]}{C_T}$ $\frac{1}{\frac{[H^+]^2}{K_1K_2} + \frac{[H^+]}{K_2} + 1}$
1	$K_1/[H^+]$	$K_1K_2/[H^+]^2$
$[H^+]/K_1$	1	$K_2/[H^+]$
$[H^+]^2/K_1K_2$	$[H^+]/K_2$	1

- If  $pH \ll pK_1$ , or  $[H^+] \gg K_1$
- If  $pK_1 \ll pH \ll pK_2$ , or  $K_1 \gg [H^+] \gg K_2$
- If  $pK_2 \ll pH$ , or  $K_2 \gg [H^+]$

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## Substances of low solubility

- Solubility product defines the limit of solubility
  - For calcium sulfate we have:

$$K_{so} = [Ca^{+2}][SO_4^{-2}] = 10^{-4.6}$$

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## Solubility

- Solubility product constants
  - The solubility product constant for the dissolution of  $\text{CaSO}_4$  is about  $10^{-4.6}$ . If you add 100 g of  $\text{CaSO}_4$  (GFW=136) to 1 liter of water, what will the calcium concentration be?
 
$$K_{so} = [\text{Ca}^{+2}][\text{SO}_4^{-2}] = 10^{-4.6}$$

$$[\text{Ca}^{+2}] = \sqrt{10^{-4.6}}$$

$$[\text{Ca}^{+2}] = 10^{-2.3} \text{ M}$$
  - If you have a solution of  $10^{-2} \text{ M}$   $\text{NaSO}_4$  which is entirely dissolved, and to this you add an excess of  $\text{CaSO}_4$  crystals, how much of the calcium sulfate will dissolve at equilibrium. Present your answer in moles per liter


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## Organic Chemistry

- Definitions & Intro
- Properties and Nomenclature
  - Alkanes
  - Alkenes
  - Alkynes
  - Alicyclics
  - Aromatics
  - Functional Groups

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## Nomenclature: Intro

Carbon can form a nearly limitless diversity of compounds. One reason for this is carbon's ability to bind covalently with itself in long chains:

$$\begin{array}{cccccccc} | & | & | & | & | & | & | & | \\ -C & -C & -C & -C & -C & -C & -C & -C- \\ | & | & | & | & | & | & | & | \end{array}$$

In the above structure, each carbon atom (C) is surrounded by four single bonds. This is a consequence of carbon's tendency to form four covalent bonds each. These extra bonds not used to join the carbon chain may be linked to hydrogen atoms or other structures. The particular structure shown above is an aliphatic chain. The carbons are linked in a linear fashion, without forming rings or cycles.

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## Nomenclature: Alkanes

### 1. Unbranched Alkanes

An homologous series of simple aliphatic organic compounds is then the following:

$\begin{array}{c} H \\   \\ H-C-H \\   \\ H \end{array}$	$\begin{array}{c} H & H \\   &   \\ H-C & -C-H \\   &   \\ H & H \end{array}$	$\begin{array}{c} H & H & H \\   &   &   \\ H-C & -C & -C-H \\   &   &   \\ H & H & H \end{array}$	$\begin{array}{c} H & H & H & H \\   &   &   &   \\ H-C & -C & -C & -C-H \\   &   &   &   \\ H & H & H & H \end{array}$	$\begin{array}{c} H & H & H & H & H \\   &   &   &   &   \\ H-C & -C & -C & -C & -C-H \\   &   &   &   &   \\ H & H & H & H & H \end{array}$
<u>Methane</u>	<u>Ethane</u>	<u>Propane</u>	<u>Butane</u>	<u>Pentane</u>

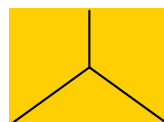
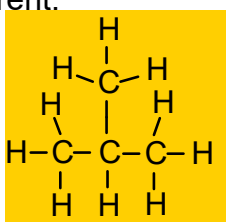
The series continues: hexane (6C), heptane (7C), octane (8C), nonane (9C), decane (10C), etc.. All alkanes have the general empirical formula,  $C_nH_{2n+2}$ .

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## Nomenclature: Branched Alkanes

### 2. Branched Alkanes & IUPAC Nomenclature

The smallest branched aliphatic is called isobutane because it is an isomer of butane (often referred to n-butane to distinguish it from isobutane). An isomer is a compound with an empirical formula identical to a second compound, but with a different structure (i.e., geometric arrangement of the atoms) is different.



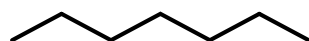
Shorthand version

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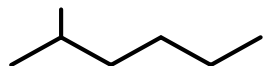
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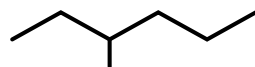
## Nomenclature: Position



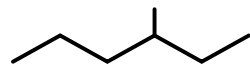
**n-Heptane**



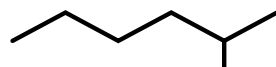
**2-Methylhexane**



**3-Methylhexane**



**3-Methylhexane**



**2-Methylhexane**

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## Nomenclature: Alkenes

### 3. Alkenes

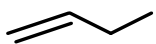
If one were to remove two hydrogens from each of the alkanes, leaving a carbon-carbon double bond in their place, one would have the series known as alkenes or olefins. Organic compounds such as these having double or triple bonds are often referred to as unsaturated, because they have less than the maximum possible number of hydrogens.



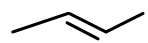
**Ethene**



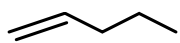
**Propene**



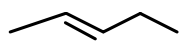
**1-Butene**



**2-Butene**



**1-Pentene**




**2-Pentene**

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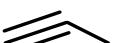
## Nomenclature: Alkynes

### 4. Alkynes

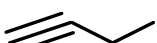
Removal of 4 hydrogens from two adjoining carbons in an alkane results in the formation of a carbon-carbon triple bond. The homologous series of these compounds is termed the alkynes (suffix -yne) and has the general empirical formula,  $C_nH_{2n-2}$ .



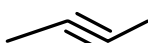
**Ethyne**



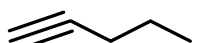
**Propyne**




**1-Butyne**



**2-Butyne**



**1-Pentyne**




**2-Pentyne**

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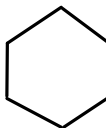
## Nomenclature: Alicyclics

5. Alicyclic Hydrocarbons

When hydrocarbon chains are joined to make a ring, they are said to be cyclic, or more properly, alicyclic. They may also have double and triple bonds (e.g., cycloalkenes, cycloalkynes, in addition to cycloalkanes). Alicyclic compounds are often given the prefix, "cyclo". These compounds have the general empirical formula,  $C_nH_{2n}$ .



**Cyclopentane**



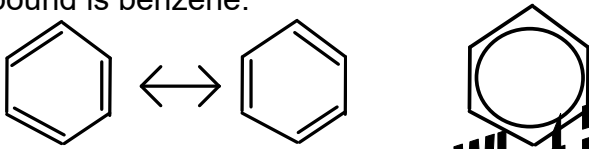
**Cyclohexane**

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## Nomenclature: Aromatics

6. Aromatics

Six-membered rings containing three alternating double and single bonds are given a special name, aromatic. These compounds are especially stable. The simplest aromatic compound is benzene.



Question: What is BTEX?

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## Aromatics

- Kekulé resonance structures of benzene

- Polynuclear (or Polycyclic) Aromatic Hydrocarbons (PAHs)

Naphthalene

Anthracene

Pyrene

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## Nomenclature: Funct. Groups 1

<u>Name</u>	<u>Structure</u>	<u>Suffix/Prefix</u>
<b>Alcohols</b>		-ol
<b>Acids</b>		-oic acid
		-ate
<b>Ketones</b>		-one
<b>Aldehydes</b>		-al
<b>Amines</b>		-yl amine

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## Nomenclature: Funct. Groups 2

<u>Name</u>	<u>Structure</u>	<u>Prefix/Suffix</u>
<b>Esters</b>	$\begin{array}{c} \text{O} \\ \parallel \\ \text{—C—O—R} \end{array}$	Alkyl(R) ___-at
<b>Ethers</b>	$\begin{array}{c} \diagup \text{C} \text{—O—} \text{C} \diagdown \\ \diagdown \quad \diagup \end{array}$	
<b>Halides</b>	$\begin{array}{c} \diagup \text{C} \text{—Cl} \\ \diagdown \\ \diagup \text{C} \text{—Br} \\ \diagdown \end{array}$	chloride bromide
<b>Amide</b>	$\begin{array}{c} \text{O} \\ \parallel \\ \text{—C—N} \\ \quad \diagdown \quad \diagup \\ \quad \text{H} \quad \text{H} \end{array}$	
<b>Nitriles</b>	$\text{—C}\equiv\text{N}$	-nitrile

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## Nomenclature question #1

■ What is this called?

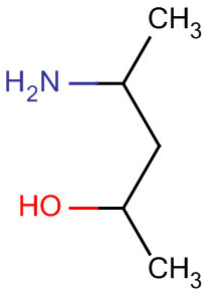
- A. Chloromethane
- B. Chlorobenzene
- C. Chlorobenzoic acid
- D. Chlorohydroxyethane
- E. None of the above

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## Nomenclature question #1

■ What is this called?

- A. 2-propanoate
- B. 1,4-hydroxybutamine
- C. Pentane-3-al
- D. 1,5-hydroxybutamine
- E. 4-amino-2-pentanol



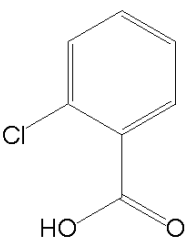
The chemical structure shows a five-carbon chain. The second carbon from the left has a hydroxyl group (HO) attached. The fourth carbon from the left has an amino group (H<sub>2</sub>N) attached. Both the hydroxyl and amino groups are highlighted in red and blue respectively. Methyl groups (CH<sub>3</sub>) are attached to the first and fifth carbons.

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## Nomenclature question #2

■ What is this called?


- A. Chloromethane
- B. Chlorobenzene
- C. Chlorobenzoic acid
- D. Chlorohydroxyethane
- E. None of the above



The chemical structure shows a benzene ring with a chlorine atom (Cl) at the 3-position and a carboxylic acid group (HO-C=O) at the 1-position.

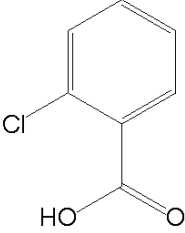
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 Nomenclature question #3

■ What is this called?

- A. 1-Chlorobenzoic acid
- B. 2-Chlorobenzoic acid
- C. 3-Chlorobenzoic acid
- D. 4-Chlorobenzoic acid
- E. 5-Chlorobenzoic acid



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 To next lecture

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