### <u>Chapter 7: Part 1:</u> Substitution Reactions - SN2

Today Chapter 7 (7.1-7.4)

- 1. Alkyl Halides
- 2. Substitution and Elimination Reactions
- 3. The SN2 Mechanism
- 4. Inversion of Configuration/ Stereochemistry
- 5. Factors Affecting SN2 Reactions
  - 1. The Leaving Group
  - 2. The Nucleophile
  - 3. Steric Hindrance
  - 4. The Solvent

### Naming Alkyl Halides



1



# Substitution and Elimination Reactions

#### In Chapters 7 -

- 2 kinds of reactions Substitution and Elimination
- Key to this understanding the factors which determine which mechanism predominates and which products form.



#### **The SN2 reaction:** Substitution Nucleophilic *Bimolecular*





(S)-(+)-2-Bromooctane

The reaction mechanism which predominates depends on the following factors:

Remember-

ctions /	Are Affected	I by the	
Leaving Group			
Relative Rate	Conjugate acid of leaving group	p <i>K</i> <sub>a</sub> of conj. acid	
<b>10</b> <sup>-5</sup>	HF	3.5	
1	HCI	-7	
10	HBr	-9	
<b>10</b> <sup>2</sup>	HI	-10	
<b>10</b> <sup>1</sup>	H <sub>3</sub> O <sup>+</sup>	-1.7	
<b>10</b> <sup>5</sup>	TsOH	-2.8	
<b>10</b> <sup>8</sup>	CF <sub>3</sub> SO <sub>2</sub> OH	-6	
	Ctions / Leavi Relative Rate 10 <sup>-5</sup> 1 10 <sup>2</sup> 10 <sup>2</sup> 10 <sup>1</sup> 10 <sup>5</sup> 10 <sup>8</sup>	ctions Are Affected Leaving Group Relative Conjugate acid of leaving group $10^{-5}$ HF 1 HCI 10 HBr $10^2$ HI $10^1$ H <sub>3</sub> O <sup>+</sup> $10^5$ TsOH $10^8$ CF <sub>3</sub> SO <sub>2</sub> OH	

A single organic product was obtained when 1-bromo-3-chloropropane was allowed to react with one molar equivalent of sodium cyanide in aqueous ethanol. What was this product?

 $BrCH_2CH_2CH_2CI + NaCN$ 

#### Nucleophilicity. What is a Nucleophile? What Makes a Good One?



## Nucleophilicity

Rank	Nucleophile	Relative
		rate
•strong	I <sup>-</sup> , HS <sup>-</sup> , RS <sup>-</sup>	>10 <sup>5</sup>
•good	Br-, HO-,	104
•	RO <sup>-</sup> , CN <sup>-</sup> , N <sub>3</sub> <sup>-</sup>	
•fair	NH <sub>3</sub> , Cl <sup>-</sup> , F <sup>-</sup> , RCO <sub>2</sub> <sup>-</sup>	10 <sup>3</sup>
•weak	$H_2O$ , ROH	1
<ul> <li>very weak</li> </ul>	$\bar{RCO_2H}$	<b>10</b> -2

- $CH_3CH_2Cl + HO^- \longrightarrow CH_3CH_2OH + Cl^$ an alcohol
- $CH_3CH_2Br + HS^- \longrightarrow CH_3CH_2SH + Br^$ a thiol

$$CH_3CH_2I + RO^- \longrightarrow CH_3CH_2OR + I^-$$
  
an ether

- $CH_3CH_2Br + RS^- \longrightarrow CH_3CH_2SR + Br^$ a thioether

$$CH_{3}CH_{2}I + \ \ \ \ C \equiv N \longrightarrow CH_{3}CH_{2}C \equiv N + I \\a \text{ nitrile}$$

S<sub>N</sub>2 Reactivity versus Type of Solvent S<sub>N</sub>2 Reaction Rates Increase in Polar Aprotic Solvents

 $CH_3CH_2CH_2CH_2Br + N_3^-$ 

- •Solvent Type Relative rate
- •CH<sub>3</sub>OH
- •H<sub>2</sub>O
- •DMSO
- •DMF
- •Acetonitrile

polar protic polar protic polar aprotic polar aprotic polar aprotic















(CH<sub>3</sub>)<sub>3</sub>CBr



CH<sub>3</sub>CH<sub>2</sub>Br

(CH<sub>3</sub>)<sub>2</sub>CHBr









# Summary of SN2

## For Next Time....

<u>WEDNESDAY Chapter 7 (7.1-7.4)</u> <u>FRIDAY Chapter 7: Alkenes and Eliminations (7.5-7.8)</u> <u>NEXT MONDAY Chapter 7: Unimolecular Reactions</u> (7.9-7.10) <u>FRIDAY Chapter 7: Putting it all together 7.11</u>

<u>Suggested Homework Problems Chapter 6</u> #4, 7, 11, 17, 24, 26, 28, 34-36

Suggested Homework Problems Chapter 7

#1,3,5,16, 18, 21, 37, 41, 47, 48, 54, 56, 60, 62-65, 70, 76