

Substitution Reactions

Course Name: General Chemistry

Course Code: CHEM F111

Lecture Instructor Name: Prof. Subhasish Roy

Department: Chemistry

Email: subhasishr@goa.bits-pilani.ac.in

Chamber No: C 223

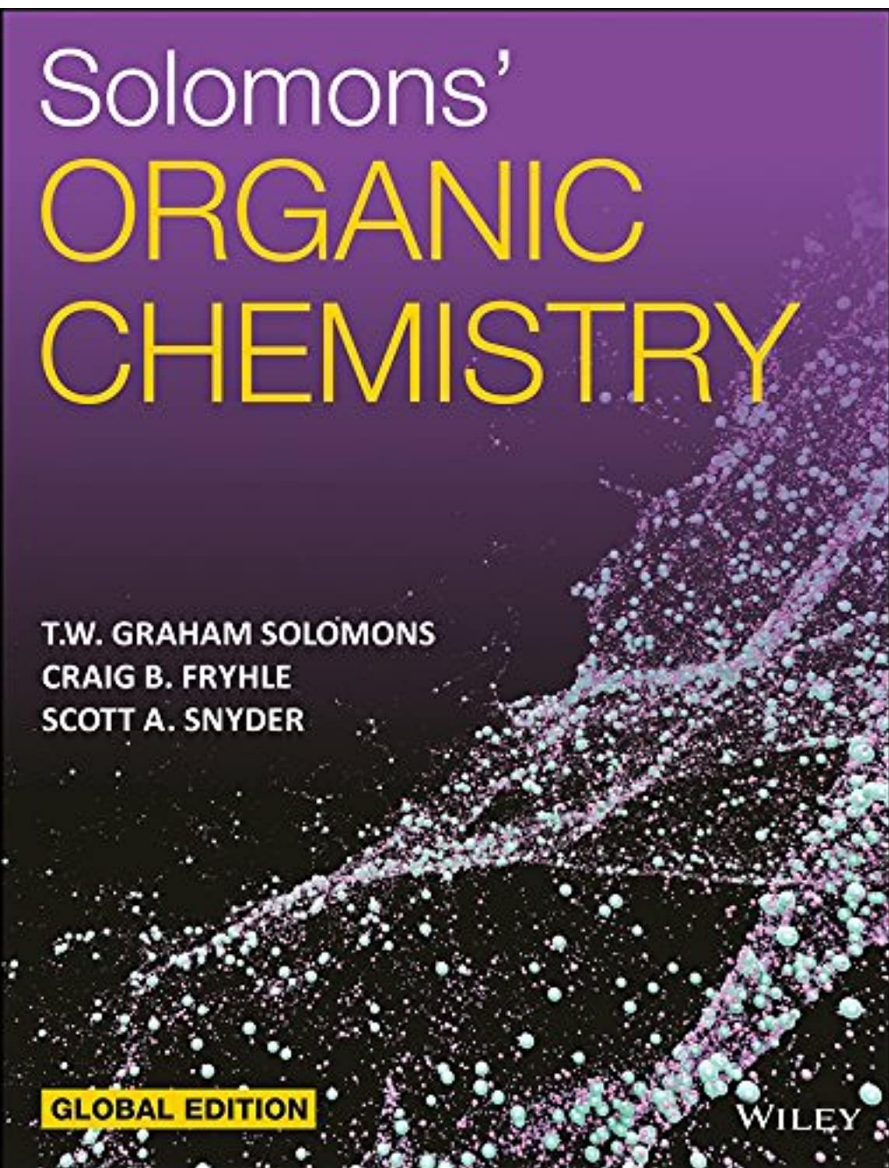
Chamber Consultation Hours: Thursday 4:00 PM to 4:50 PM

Substitution Reactions

Contents:

- 6.2 Nucleophilic Substitution Reactions
- 6.3 Nucleophiles
- 6.4 Leaving Groups
- 6.5 Kinetics of a Nucleophilic Substitution Reaction: An S_N2 Reaction
- 6.6 A Mechanism for the S_N2 Reaction
- 6.7 Transition State Theory: Free-Energy Diagrams
- 6.8 The Stereochemistry of S_N2 Reactions
- 6.9 The Reaction of Tert-Butyl Chloride with Water: An S_N1 Reaction
- 6.10 A Mechanism for the S_N1 Reaction
- 6.11 Carbocations
- 6.12 The Stereochemistry of S_N1 Reactions
- 6.13 Factors Affecting the Rates of S_N1 and S_N2 Reactions
- 6.14 Organic Synthesis: Functional Group Transformations Using S_N2 Reactions

Text Book



Most of the Lecture Slides are made from the course text book. I am gratefully acknowledging Solomon's Organic Chemistry Book and many other Organic Chemistry Books.

6.2 Nucleophilic Substitution Reactions

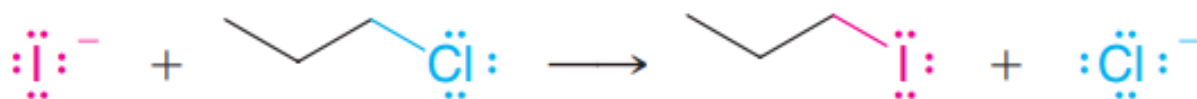


The nucleophile is a Lewis base that donates an electron pair to the substrate.

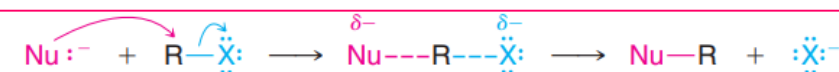
The bond between the carbon and the leaving group breaks, giving both electrons from the bond to the leaving group.

The nucleophile uses its electron pair to form a new covalent bond with the substrate carbon.

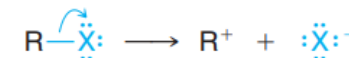
The leaving group gains the pair of electrons that originally bonded it in the substrate.



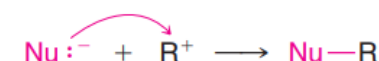
- 1 The nucleophile is always a Lewis base, and it may be negatively charged or neutral.
- 2 The leaving group is always a species that takes a pair of electrons with it when it departs.



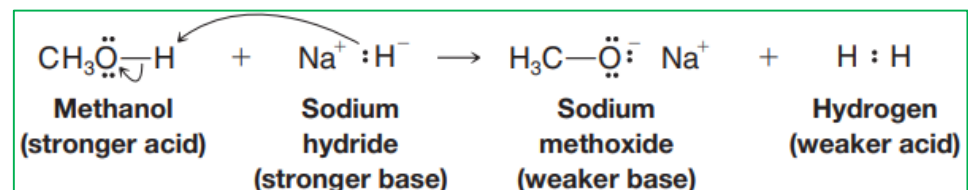
Or, does the bond to the leaving group break first?



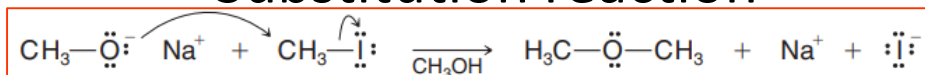
Followed by



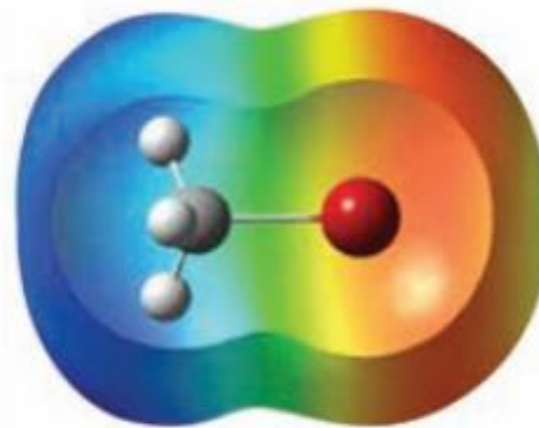
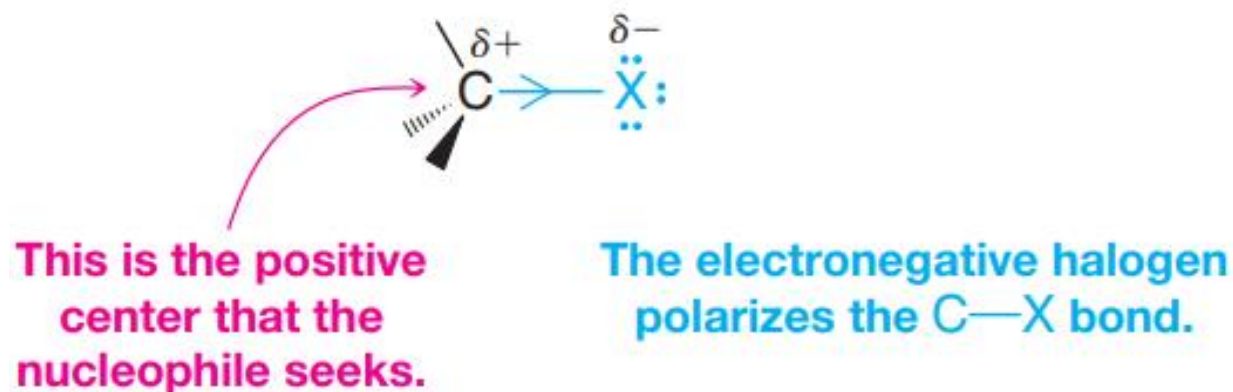
Acid-base reaction



Substitution reaction



When a nucleophile reacts with an alkyl halide, the carbon atom bearing the halogen atom is the positive center that attracts the nucleophile. This carbon carries a partial positive charge because the electronegative halogen pulls the electrons of the carbon–halogen bond in its direction.

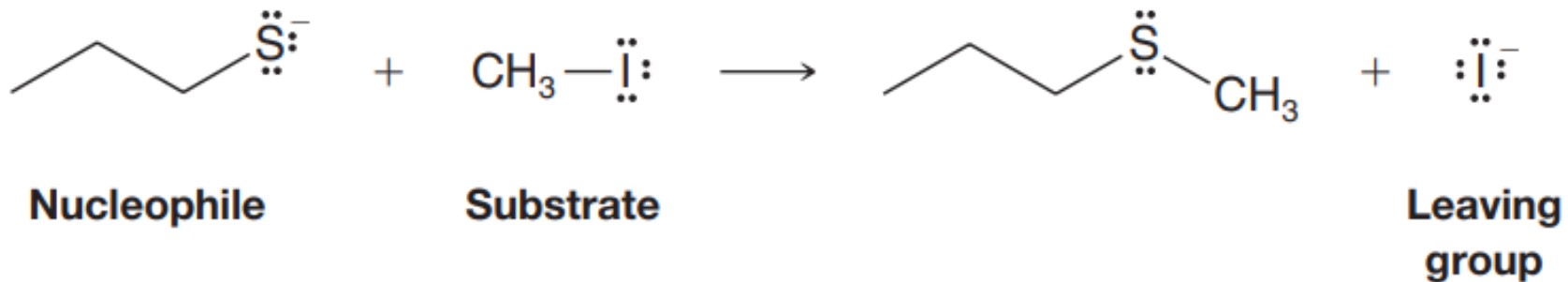


- ☞ In nucleophilic substitution reactions the bond between the substrate carbon and the leaving group undergoes *heterolytic bond cleavage*.
- ☞ The unshared electron pair of the nucleophile forms the new bond to the carbon atom.
- ☞ A key question we shall want to address later in this chapter is this: **when does the bond between the leaving group and the carbon break?**
- ☞ **Does it break at the same time that the new bond between the nucleophile and carbon forms, as shown in the previous slide?**

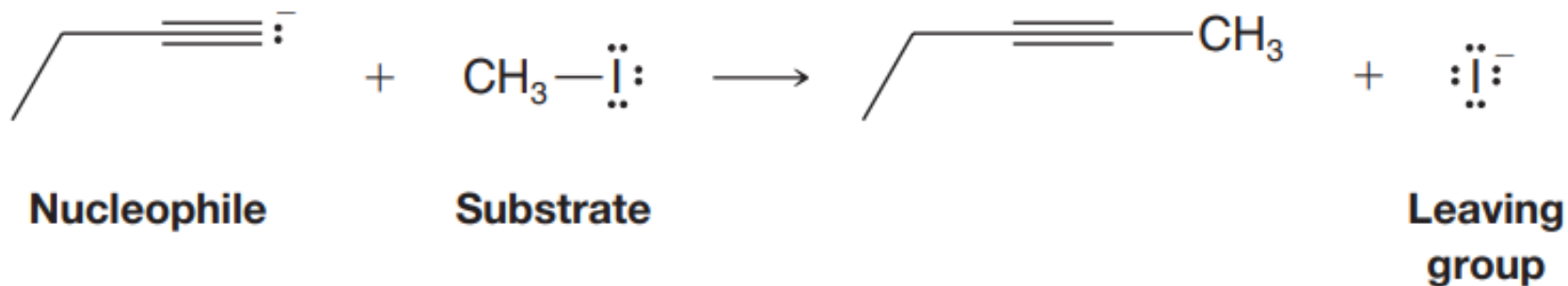
6.3 Nucleophiles

Any negative ion or uncharged molecule with an unshared electron pair is a potential nucleophile.

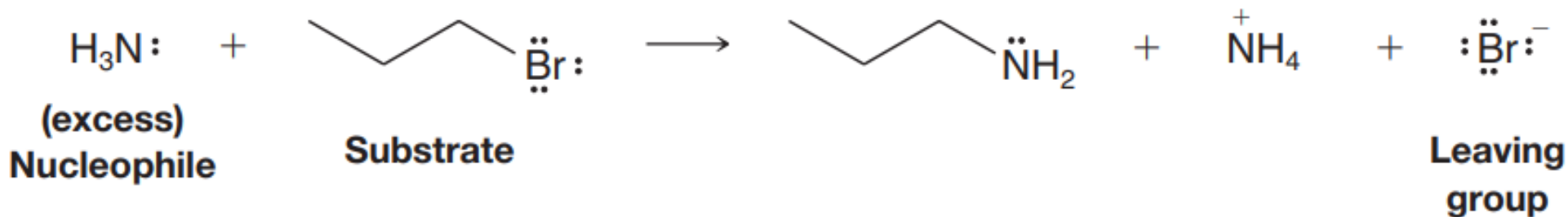
(a)



(b)



(c)

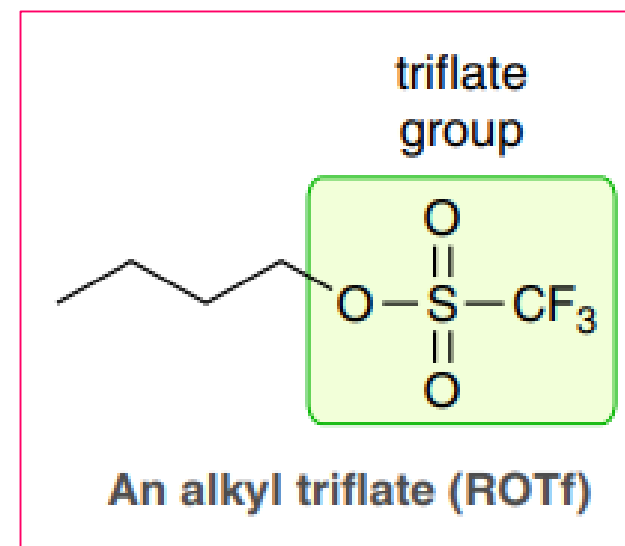
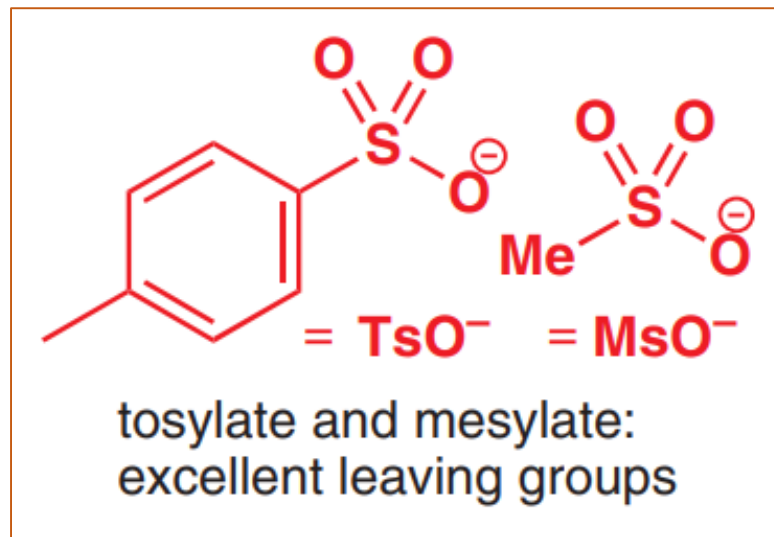
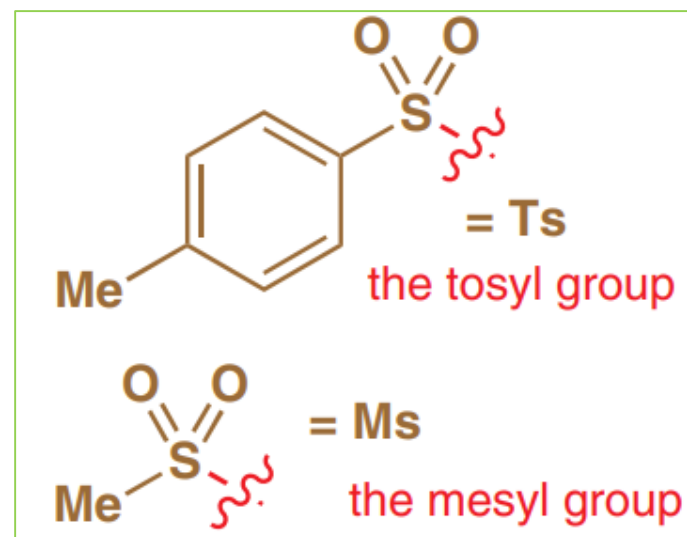


6.4 Leaving Group

□ A good leaving group is a substituent that can leave as a relatively stable, weakly basic molecule or ion.

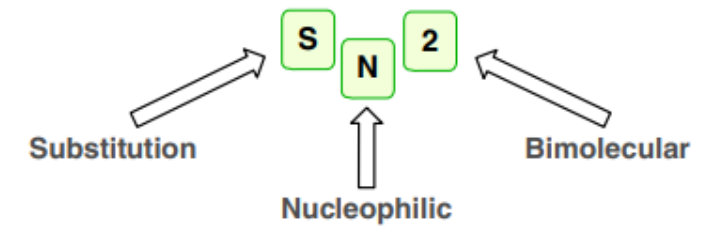
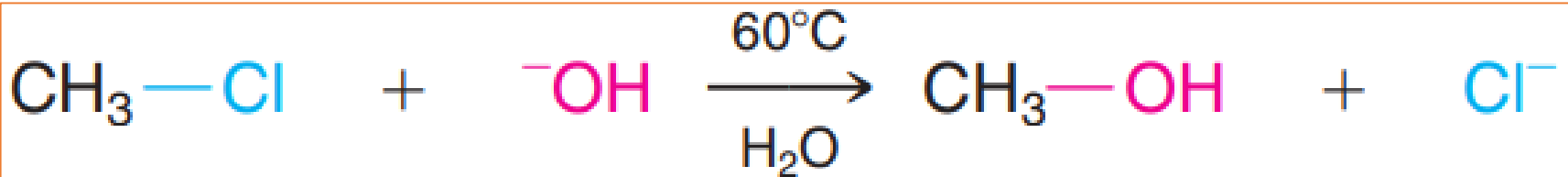
Relative reactivity	$\text{OH}^-, \text{NH}_2^-, \text{OR}^-$	F^-	Cl^-	Br^-	I^-	TosO^-
	$\ll 1$	1	200	10,000	30,000	60,000

Leaving group reactivity



6.5 Kinetics of a Nucleophilic Substitution Reaction: An S_N2 Reaction

□ A good leaving group is a substituent that can leave as a relatively stable, weakly basic molecule or ion.



RATE STUDY OF REACTION OF CH₃Cl WITH HO[−] AT 60 °C

Experiment Number	Initial [CH ₃ Cl]	Initial [HO [−]]	Initial Rate (mol L ^{−1} s ^{−1})
1	0.0010	1.0	4.9 × 10 ^{−7}
2	0.0020	1.0	9.8 × 10 ^{−7}
3	0.0010	2.0	9.8 × 10 ^{−7}
4	0.0020	2.0	19.6 × 10 ^{−7}

$$\text{Rate} \propto [\text{CH}_3\text{Cl}][\text{HO}^-]$$

$$\text{Rate} = k[\text{CH}_3\text{Cl}][\text{HO}^-]$$

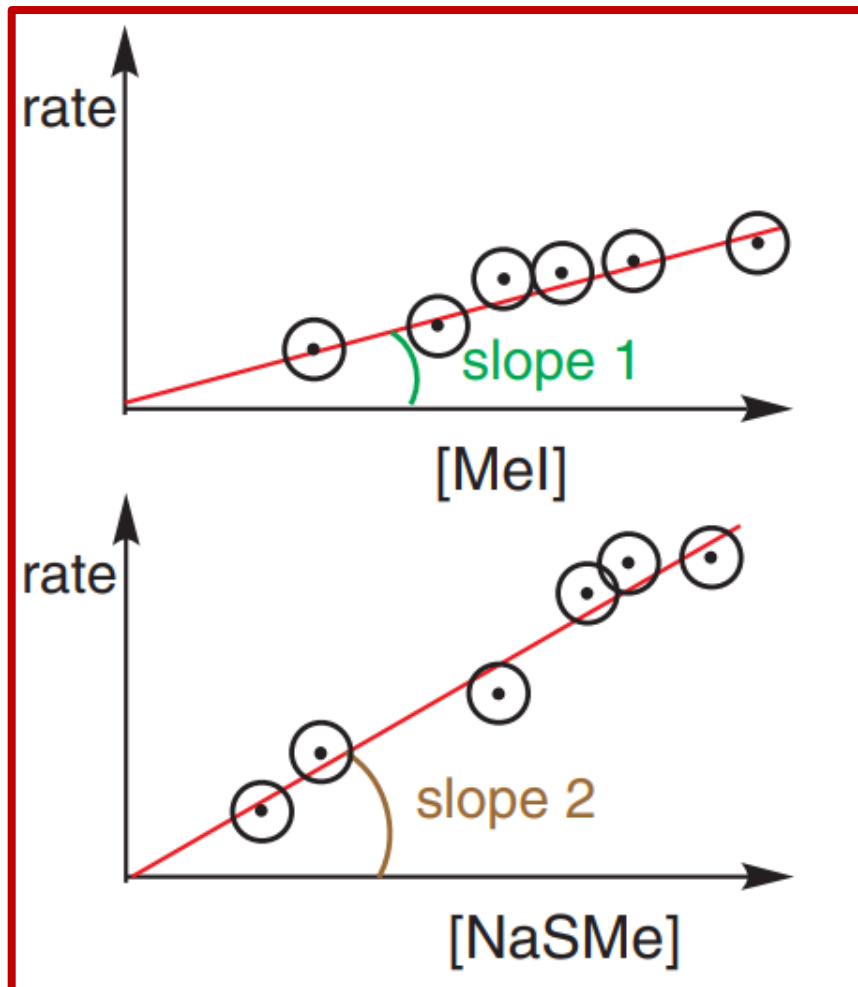
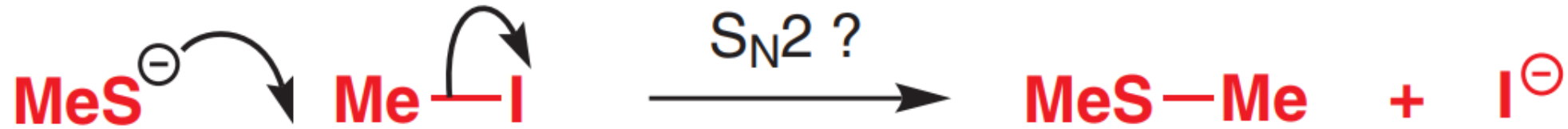
Notice that the experiments show that the rate depends on the **concentration of both chloromethane and on the concentration of hydroxide ion**.

🌀 When we *doubled the concentration of chloromethane in experiment 2*, **the rate doubled**.

🌀 When we doubled the concentration of hydroxide ion in experiment 3, the rate doubled.

🌀 **When we doubled both concentrations in experiment 4, the rate increased by a factor of four.**

6.5 Kinetics of a Nucleophilic Substitution Reaction: An S_N2 Reaction



$$\text{rate} = k_2 [\text{MeSNa}] [\text{MeI}]$$

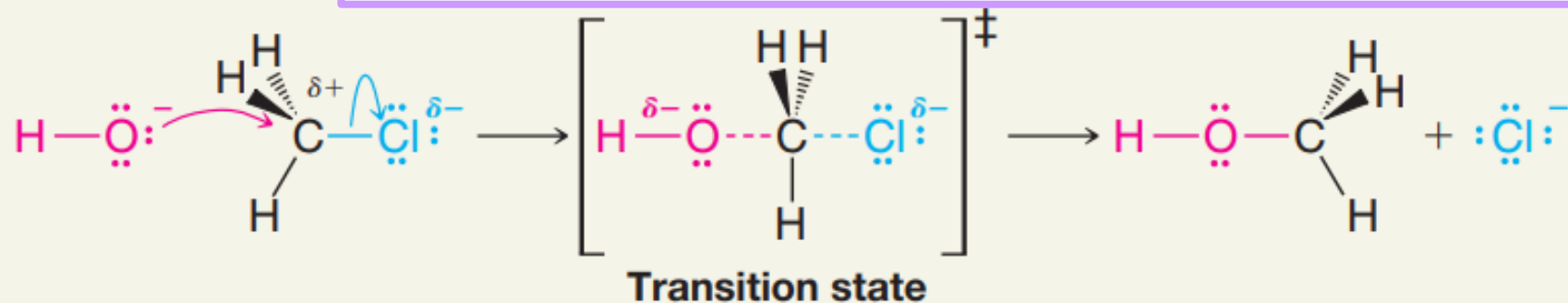
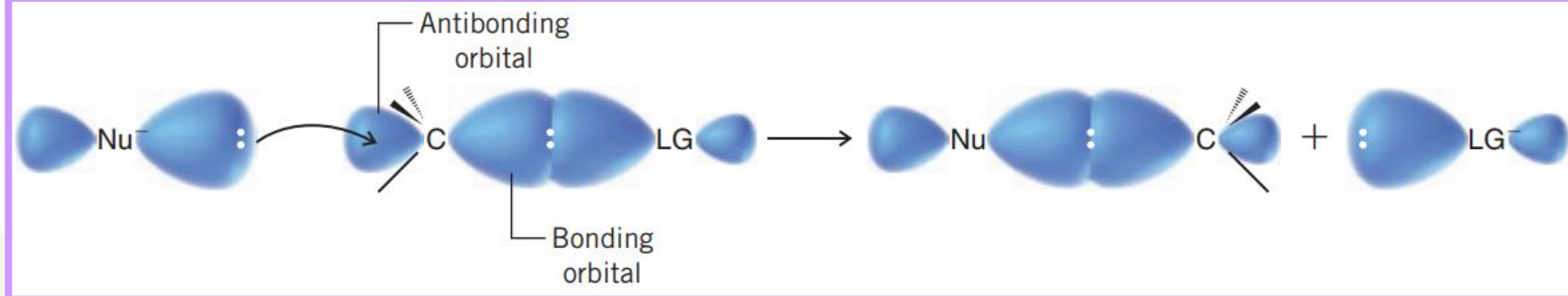
● The rate of an S_N2 reaction depends on:

- the nucleophile
- the carbon skeleton
- the leaving group

along with the usual factors of temperature and solvent.

6.6 A Mechanism for the S_N2 Reaction

Mechanism

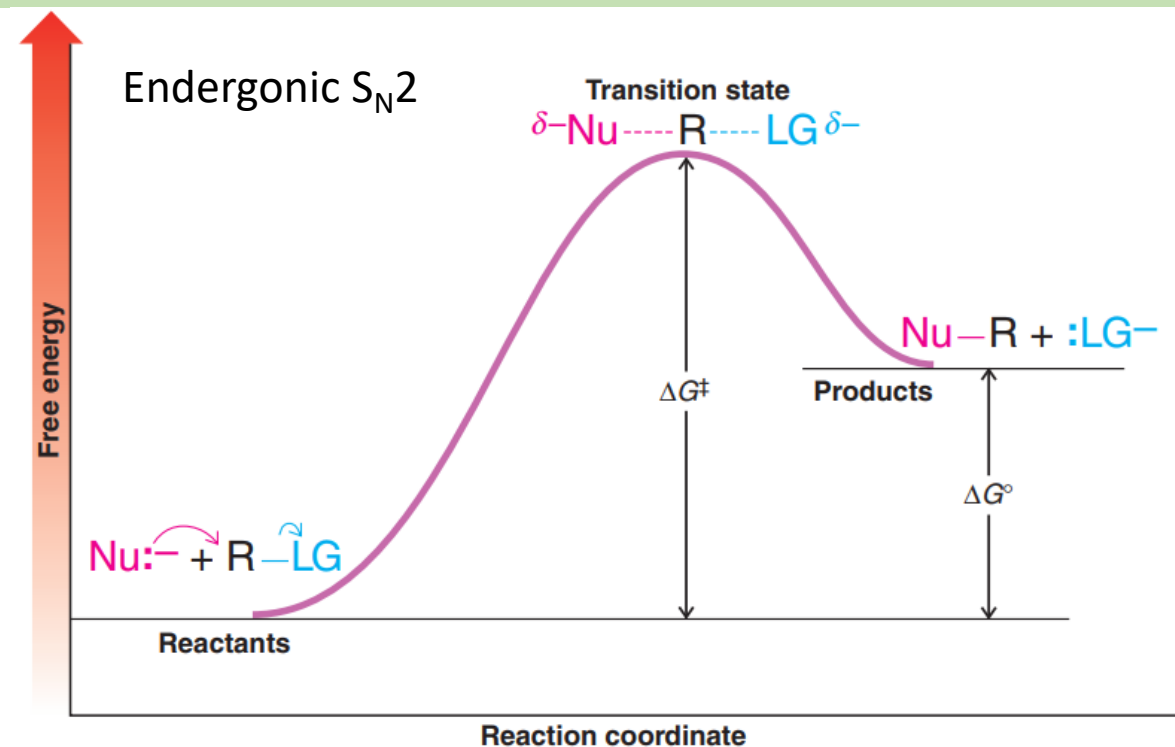
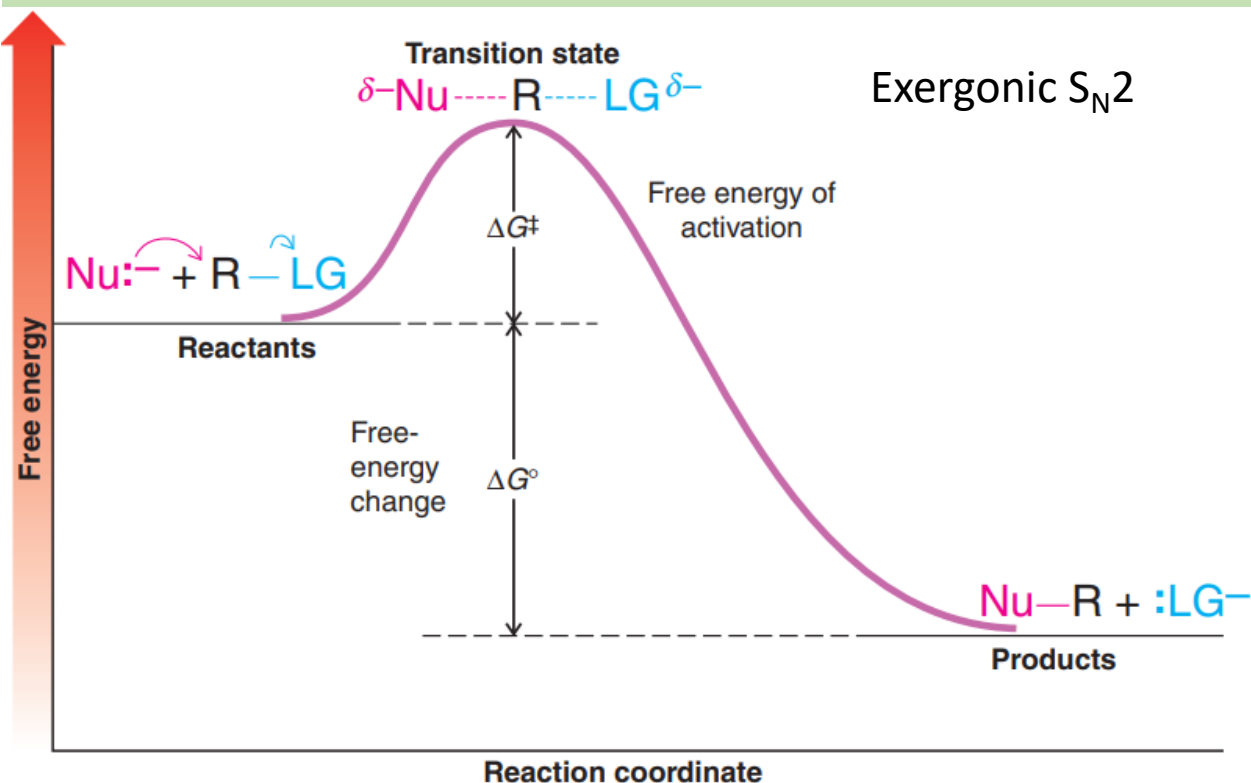


The negative hydroxide ion brings a pair of electrons to the partially positive carbon from the back side with respect to the leaving group. The chlorine begins to move away with the pair of electrons that bonded it to the carbon.

In the transition state, a bond between oxygen and carbon is partially formed and the bond between carbon and chlorine is partially broken. The configuration of the carbon atom begins to invert.

Now the bond between the oxygen and carbon has formed and the chloride ion has departed. The configuration of the carbon has inverted.

6.7 A free-energy diagram for S_N2 reaction

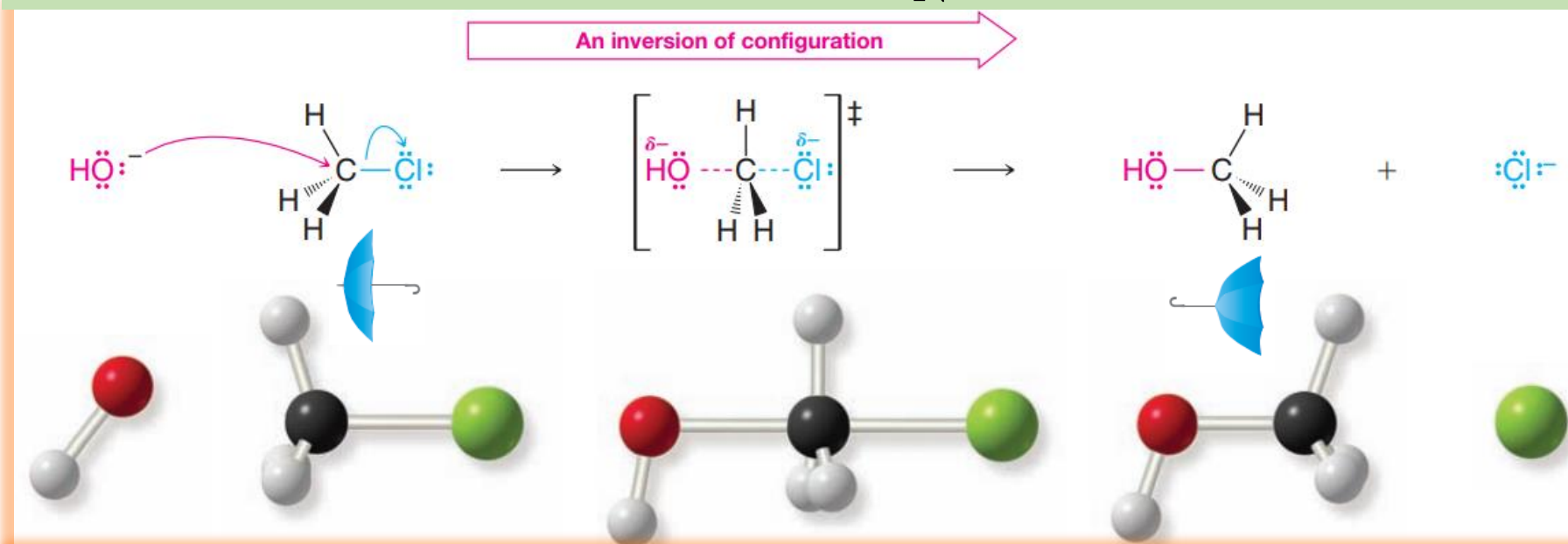


- A reaction that proceeds with a negative free-energy change (releases energy to its surroundings) is said to be **exergonic**; one that proceeds with a positive free-energy change (absorbs energy from its surroundings) is said to be **endergonic**.

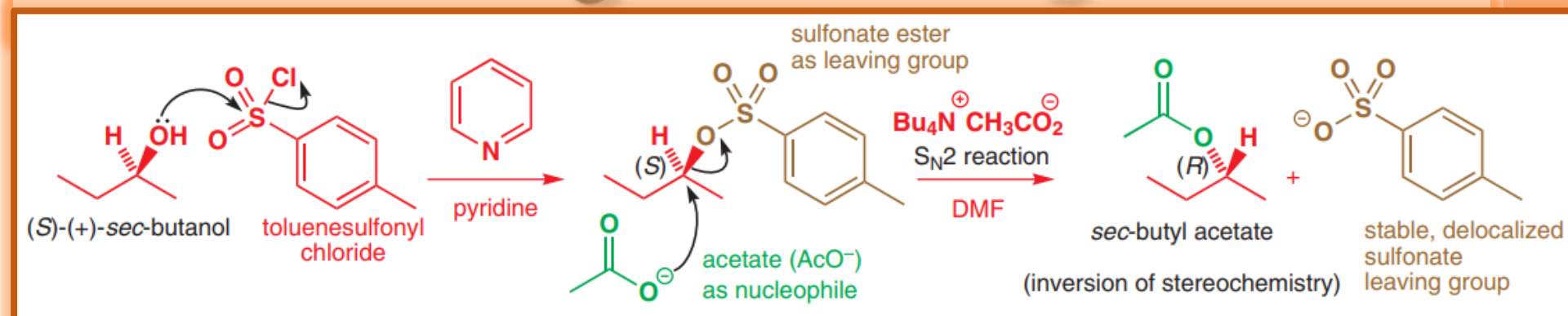
6.7A Temperature and Reaction Rate

A 10 °C increase in temperature will cause the reaction rate to double for many reactions taking place near room temperature.

6.8 The Stereochemistry of S_N2 Reactions: Inversion of Configuration

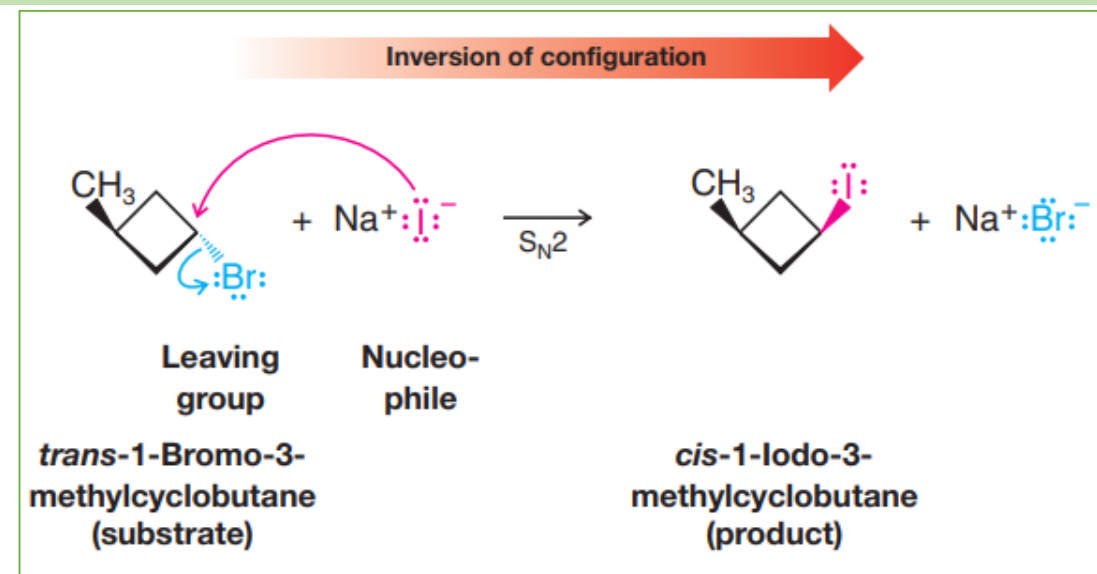
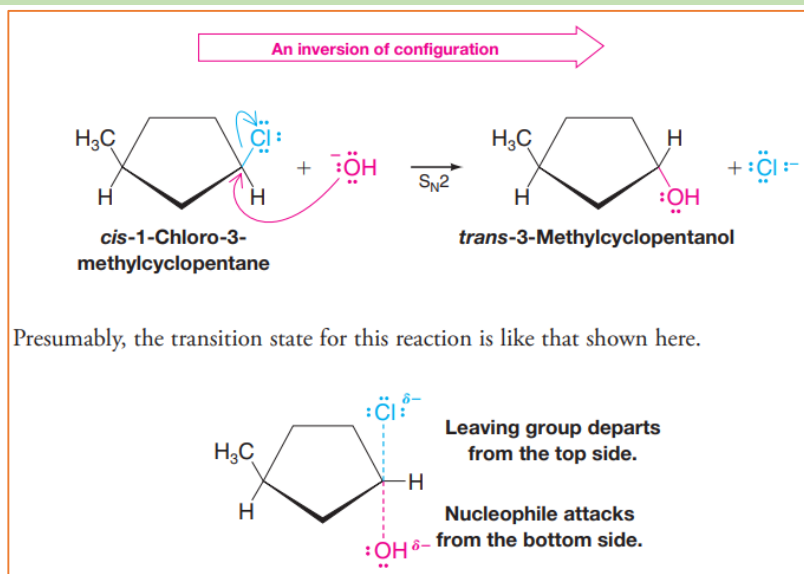


Walden inversions: The first observation of such an inversion was made by the Latvian chemist *Paul Walden* in 1896, and such inversions are called Walden inversions in his honor.

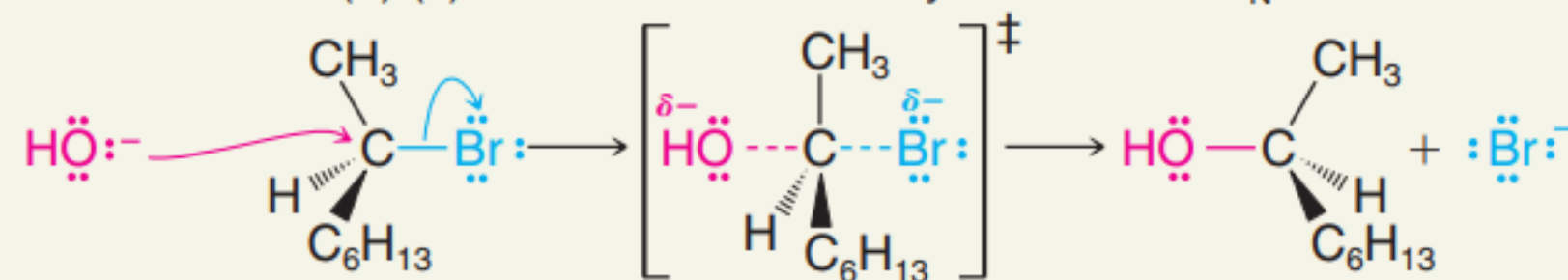


Inversion of (S)-(+)-sec-butanol to (R)-(-)-sec-butanol : An example that portrayed that ⁻OH is not a good leaving group however, it is possible to make good leaving group by converting to -OTs.

6.8 The Stereochemistry of S_N2 Reactions



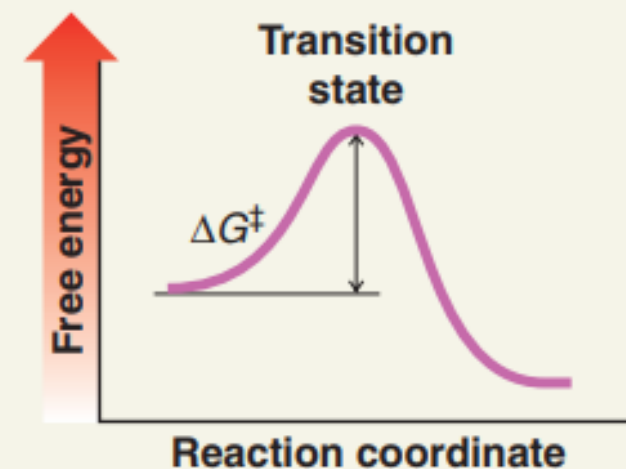
The reaction of (*R*)-(-)-2-bromooctane with hydroxide is an S_N2 reaction and takes place with *inversion of configuration*:



An inversion of configuration

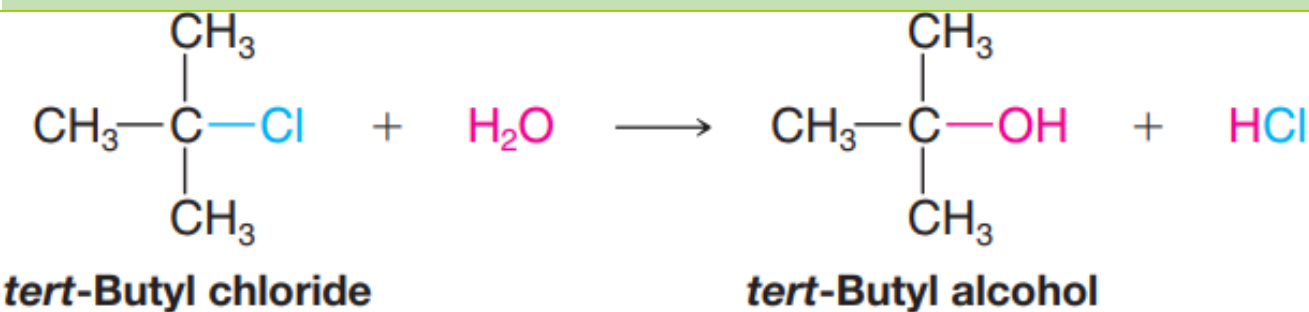
(*R*)-(-)-2-Bromooctane
 $[\alpha]_{\text{D}}^{25} = -34.25^\circ$
 Enantiomeric purity = 100%

(*S*)-(1)-2-Octanol
 $[\alpha]_{\text{D}}^{25} = +9.90^\circ$
 Enantiomeric purity = 100%



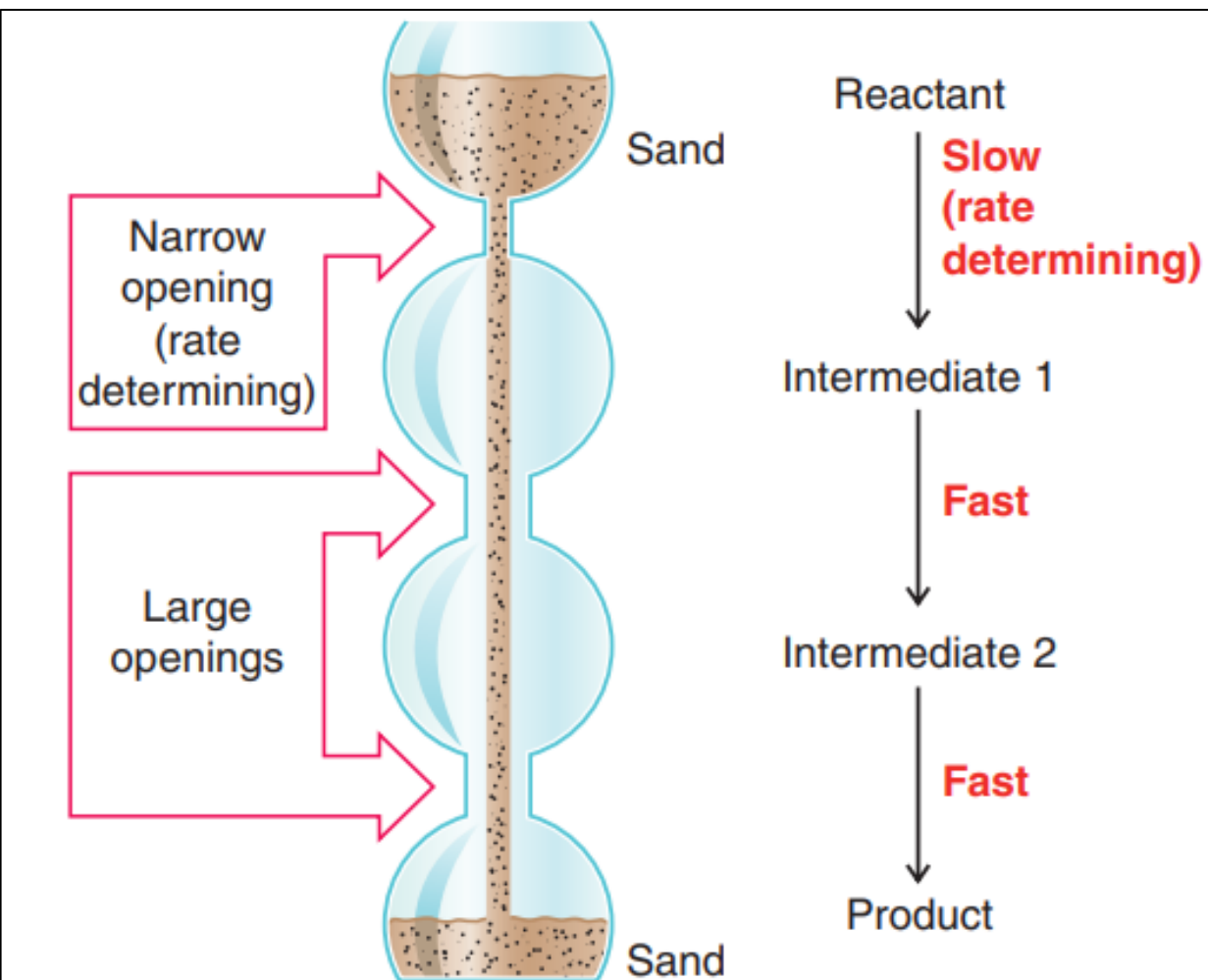
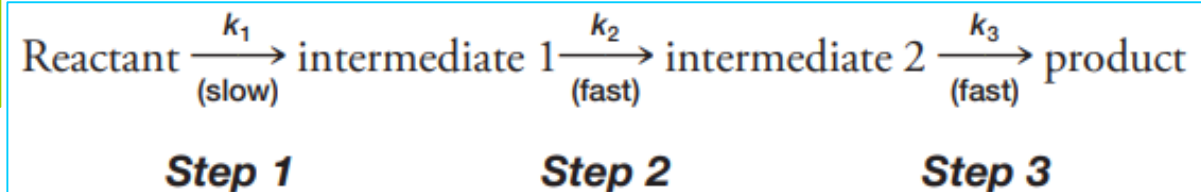
An S_N2 reaction has one transition state.

6.9 THE REACTION OF *tert*-BUTYL CHLORIDE WITH WATER: An S_N1 REACTION

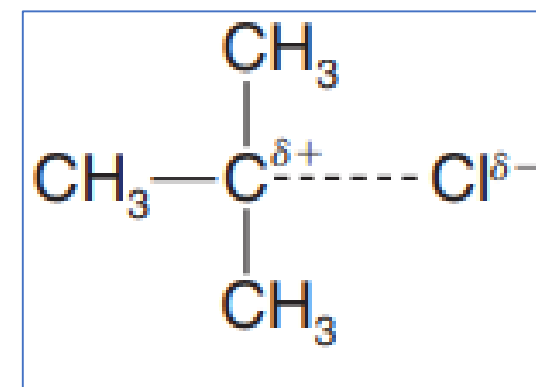
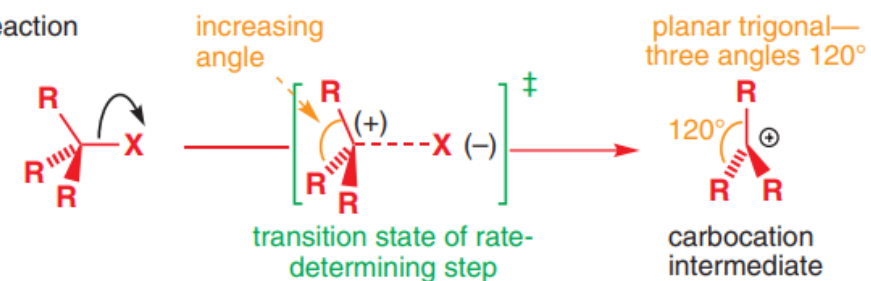


$$\text{Rate} = k[(\text{CH}_3)_3\text{CCl}]$$

The reaction rate is first order in *tert*-butyl chloride and first order overall.

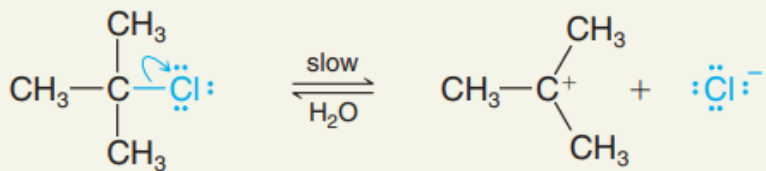


steric acceleration in the S_N1 reaction



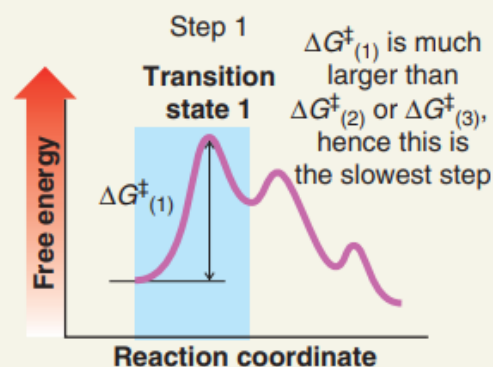
6.10 A Mechanism for the S_N1 Reaction

Step 1

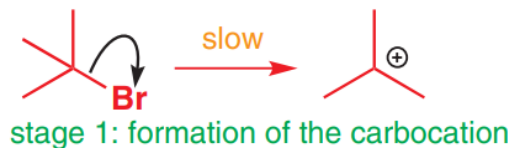


Aided by the polar solvent, a chlorine departs with the electron pair that bonded it to the carbon.

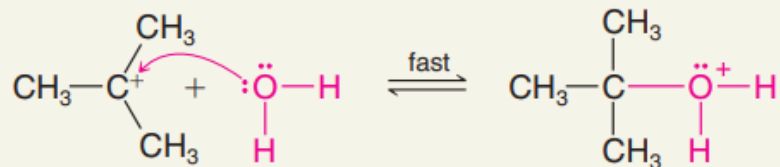
This slow step produces the 3° carbocation intermediate and a chloride ion. Although not shown here, the ions are solvated (and stabilized) by water molecules.



the S_N1 mechanism: reaction of *t*-BuBr with hydroxide ion

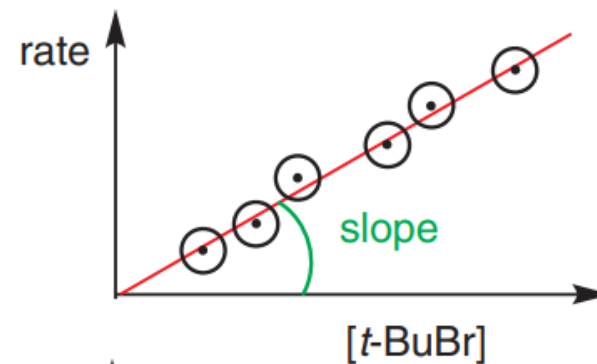
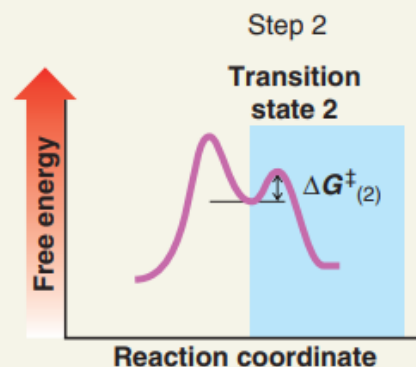


Step 2

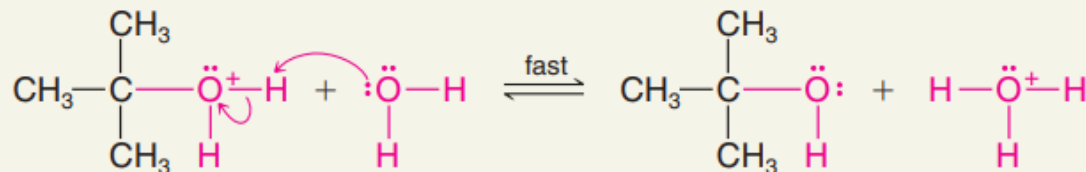


A water molecule acting as a Lewis base donates an electron pair to the carbocation (a Lewis acid). This gives the cationic carbon eight electrons.

The product is a *tert*-butyloxonium ion (or protonated *tert*-butyl alcohol).

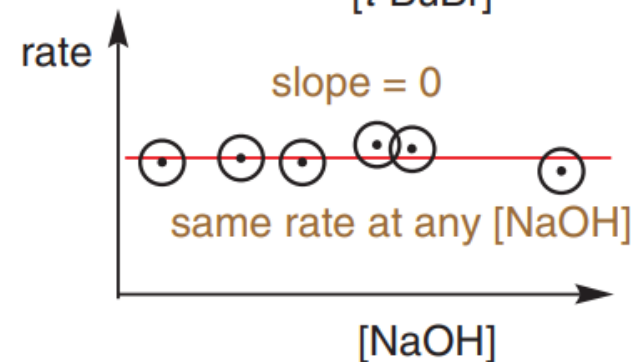
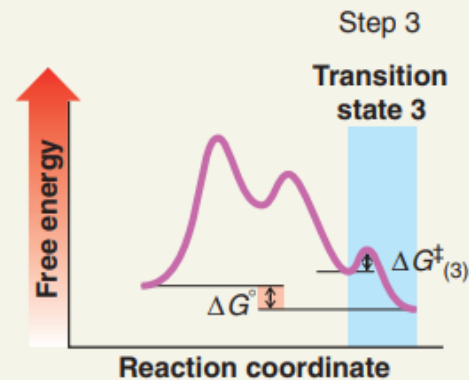


Step 3

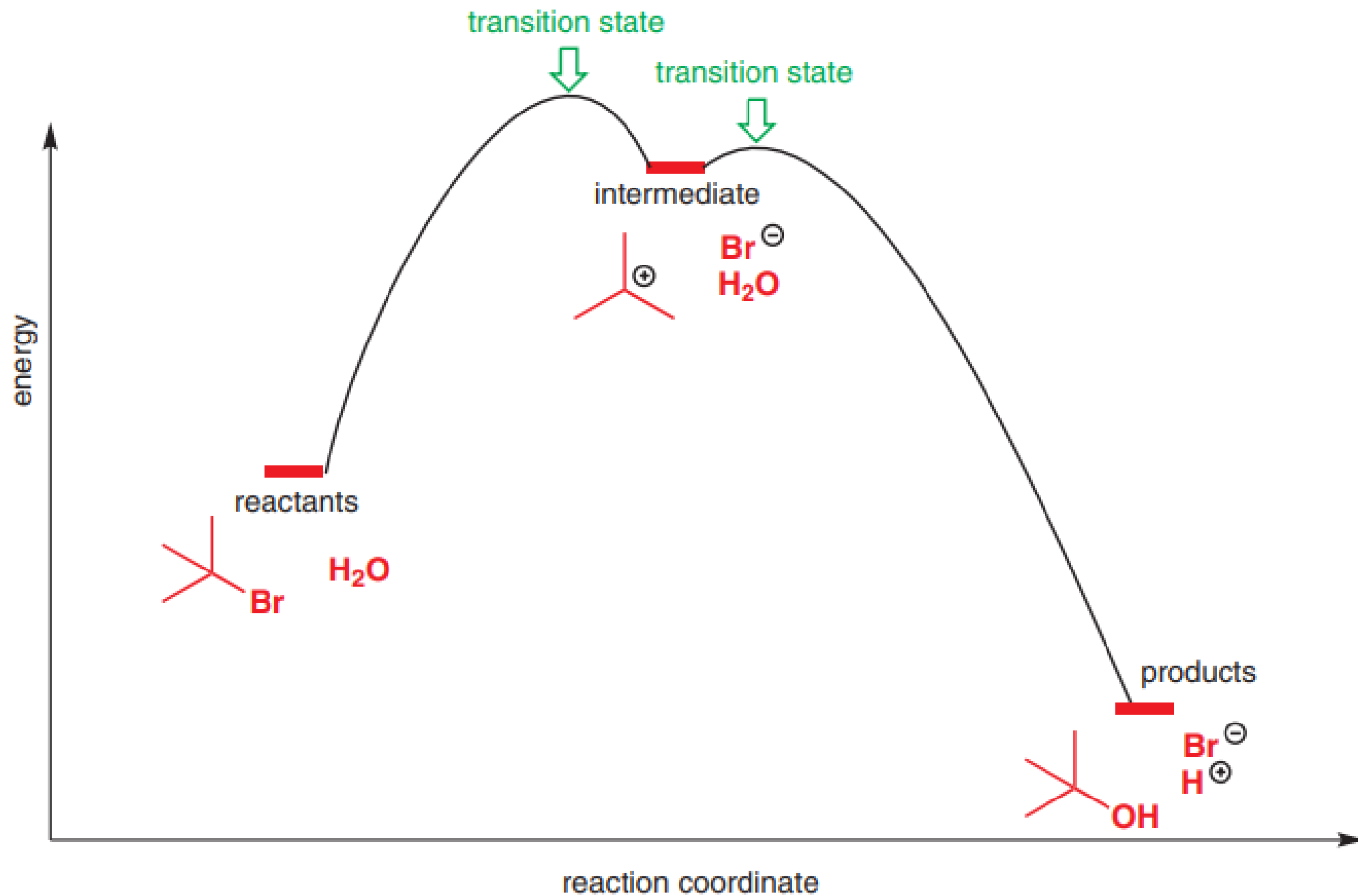


A water molecule acting as a Brønsted base accepts a proton from the *tert*-butyloxonium ion.

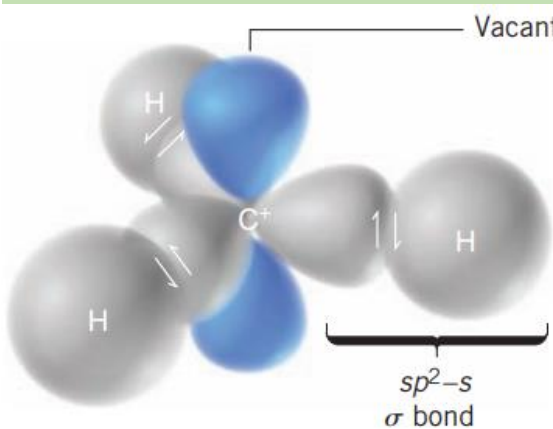
The products are *tert*-butyl alcohol and a hydronium ion.



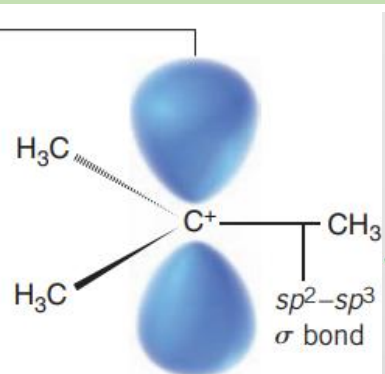
6.10 S_N1 Reaction Energy Diagram



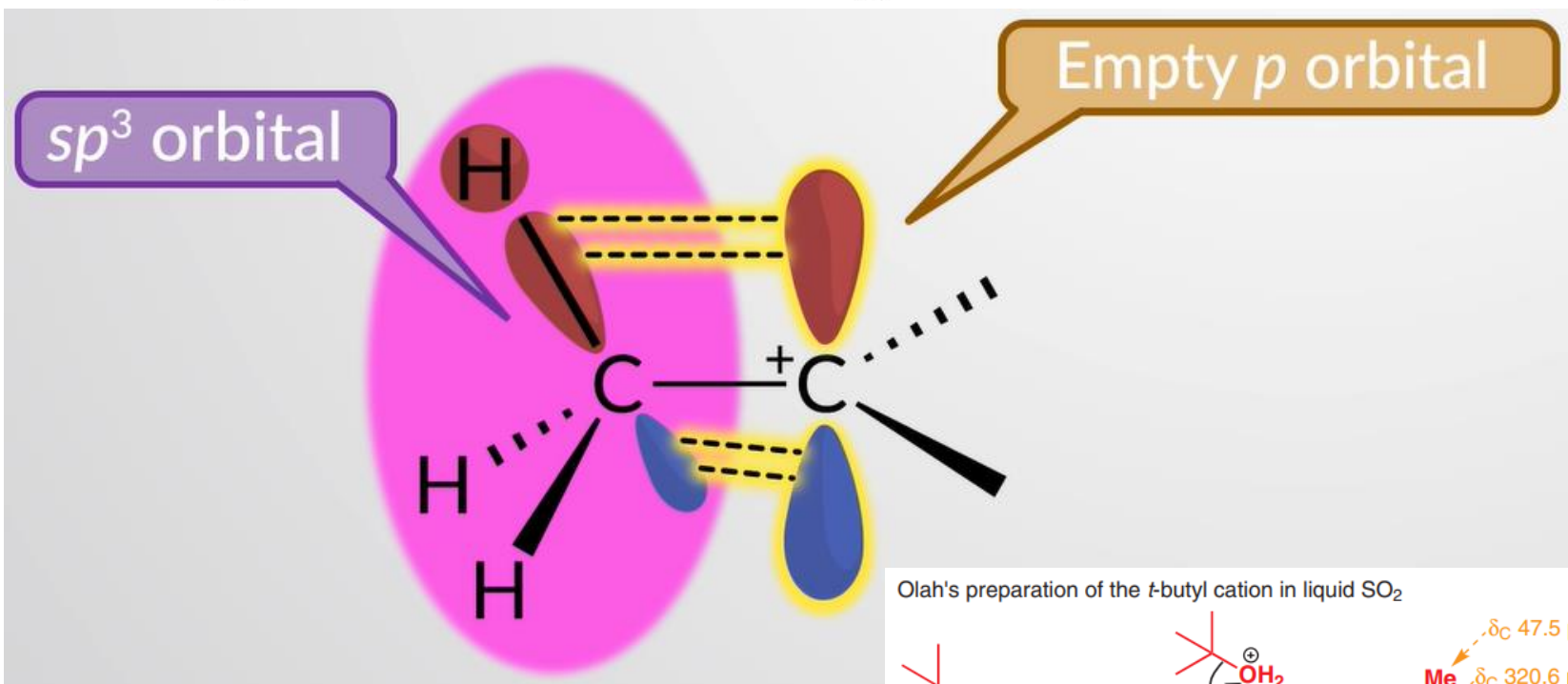
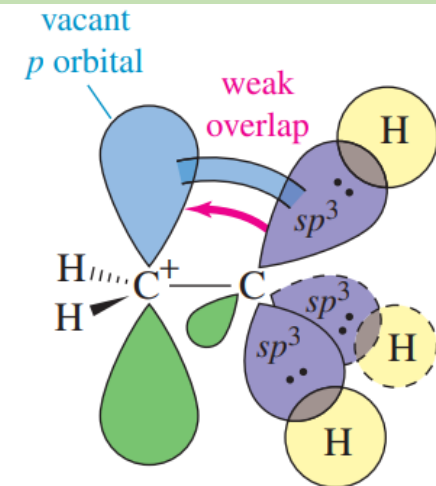
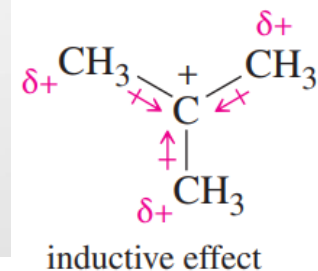
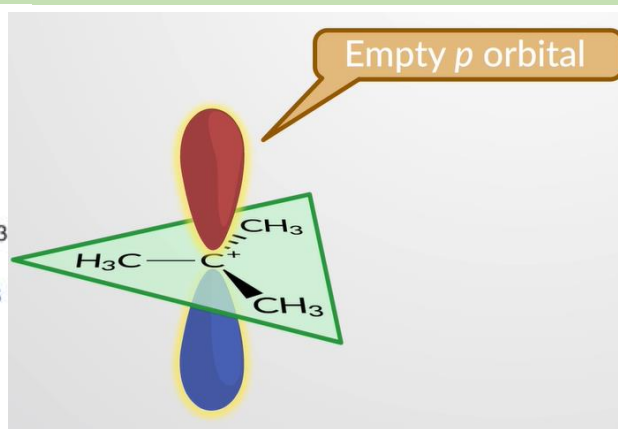
6.11 Carbocations



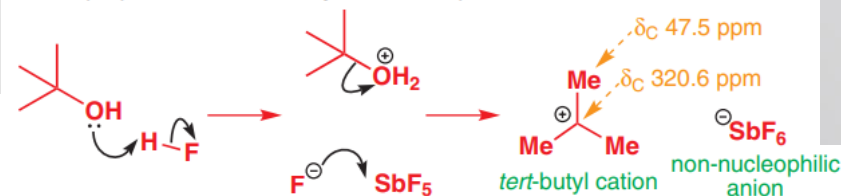
(a)



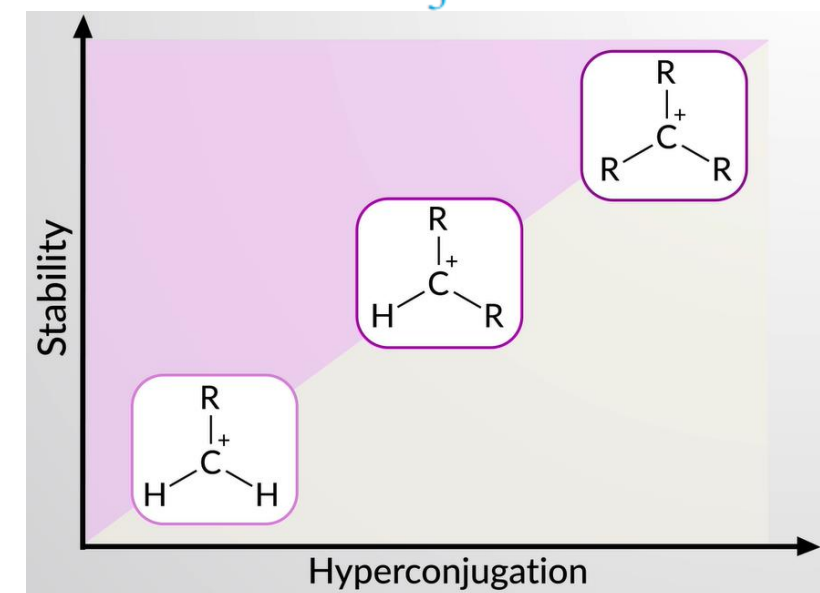
(b)



Olah's preparation of the *t*-butyl cation in liquid SO_2

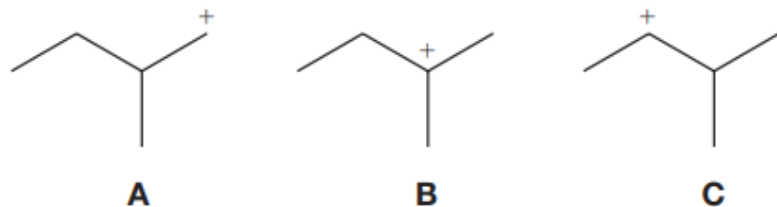


carbocation stability:
 $3^\circ > 2^\circ > 1^\circ > ^+CH_3$

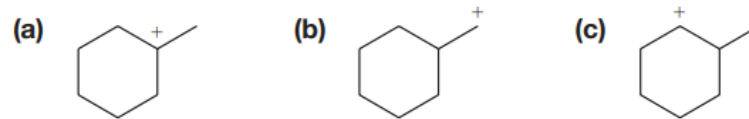


6.11 Stability of Carbocations

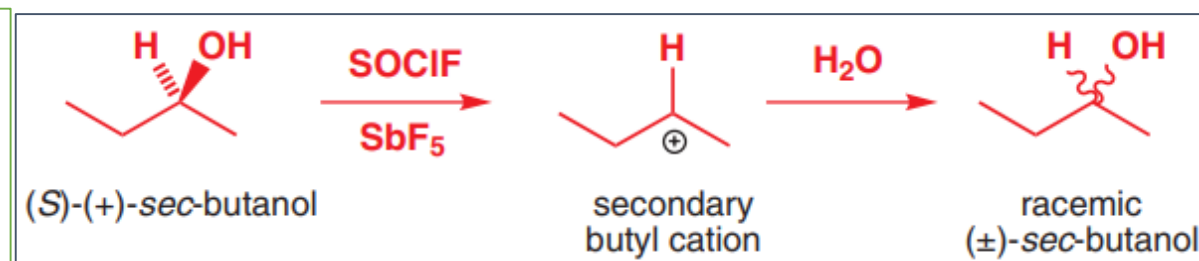
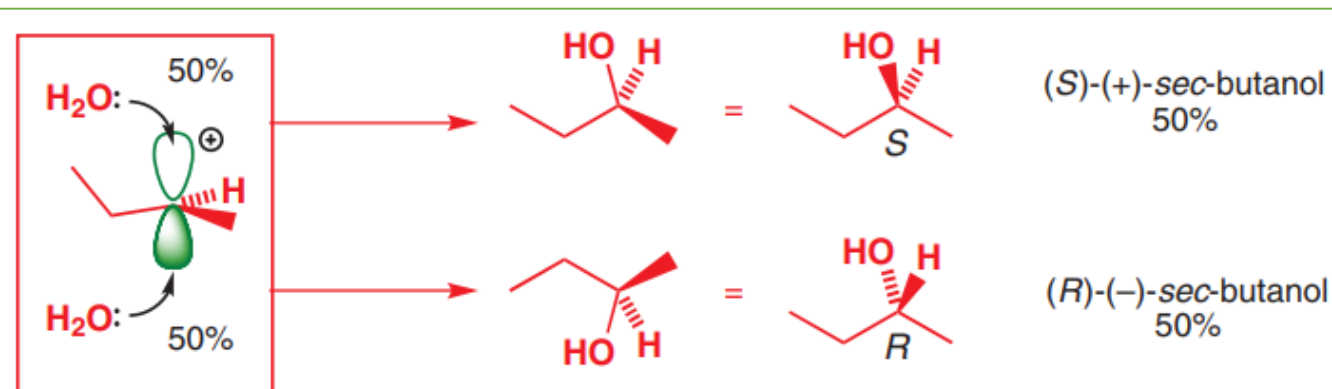
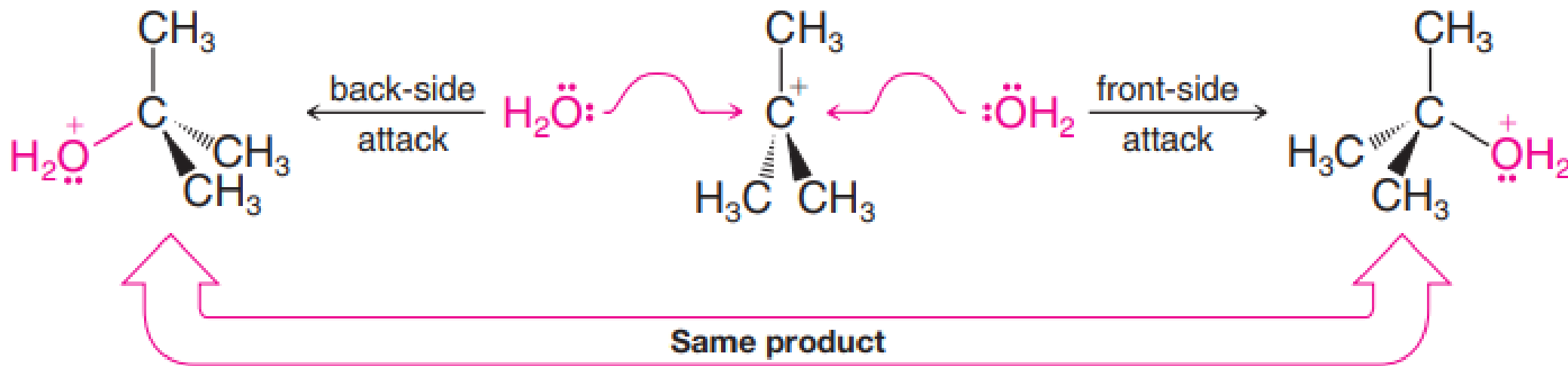
Rank the following carbocations in order of increasing stability:



PRACTICE PROBLEM 6.7 Rank the following carbocations in order of increasing stability:



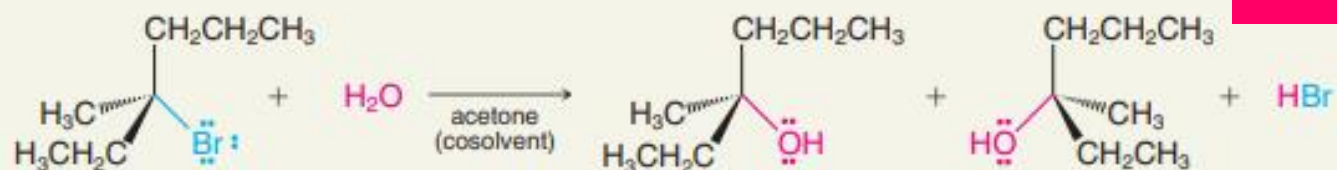
6.12 The Stereochemistry of S_N1 Reaction



SOCIF = Thionyl chloride fluoride

6.12A Reactions That Involve Racemization

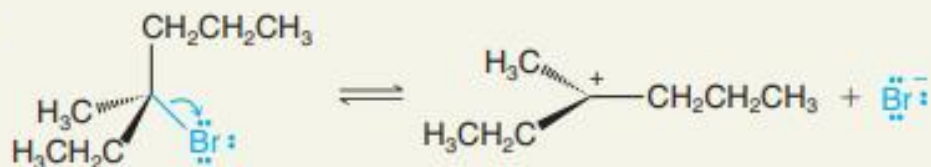
Reaction



Mechanism

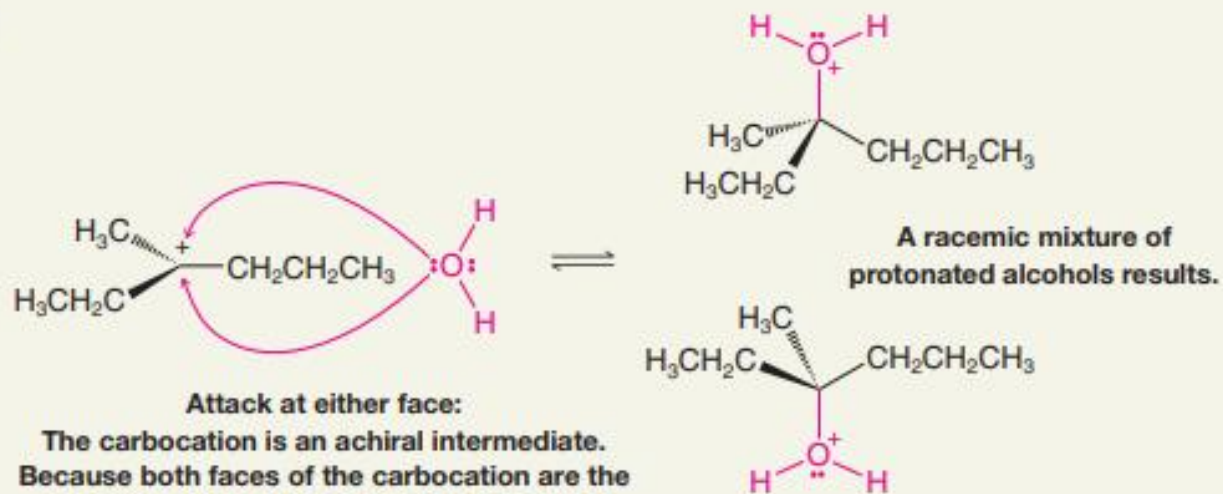
Mechanism

Step 1

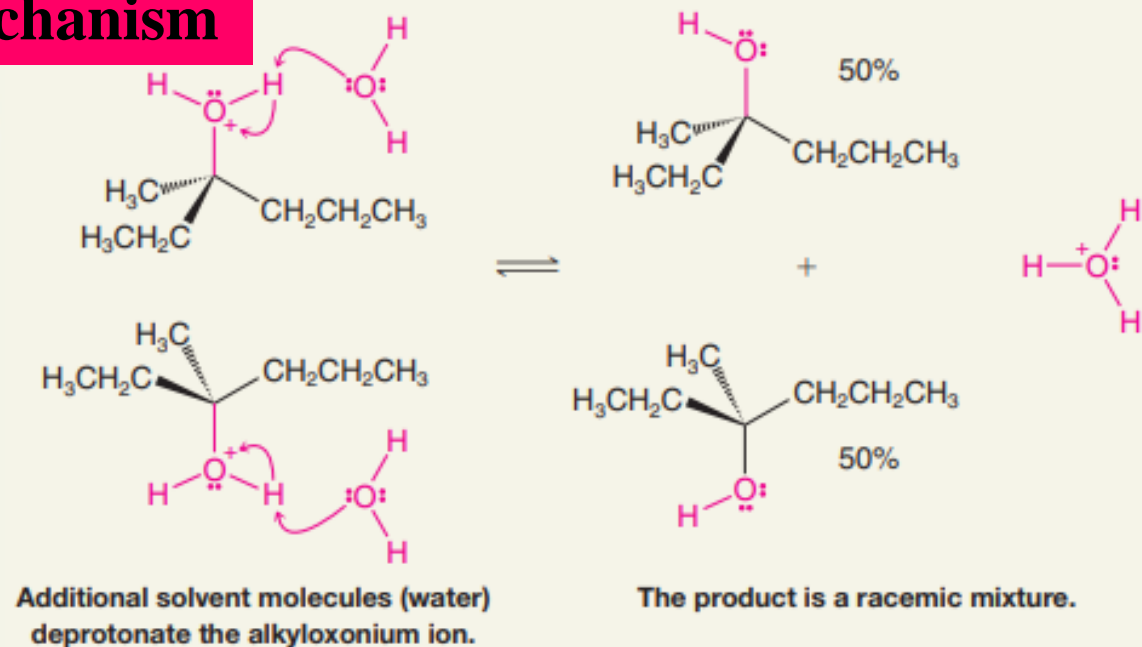


Departure of the leaving group (assisted by hydrogen bonding with water) leads to the carbocation.

Step 2



Attack at either face:
The carbocation is an achiral intermediate. Because both faces of the carbocation are the same, the nucleophile can bond with either face to form a mixture of stereoisomers.



Racemic Mixtures:
 \pm , 50 : 50 enantiomeric mixtures

6.13 Factors Affecting the Rates of S_N1 and S_N2 Reactions

□ A number of factors affect the relative rates of S_N1 and S_N2 reactions.

□ The most important factors are:

1. the structure of the substrate,
2. the concentration and reactivity of the nucleophile (for S_N2 reactions only),
3. the effect of the solvent, and
4. the nature of the leaving group.

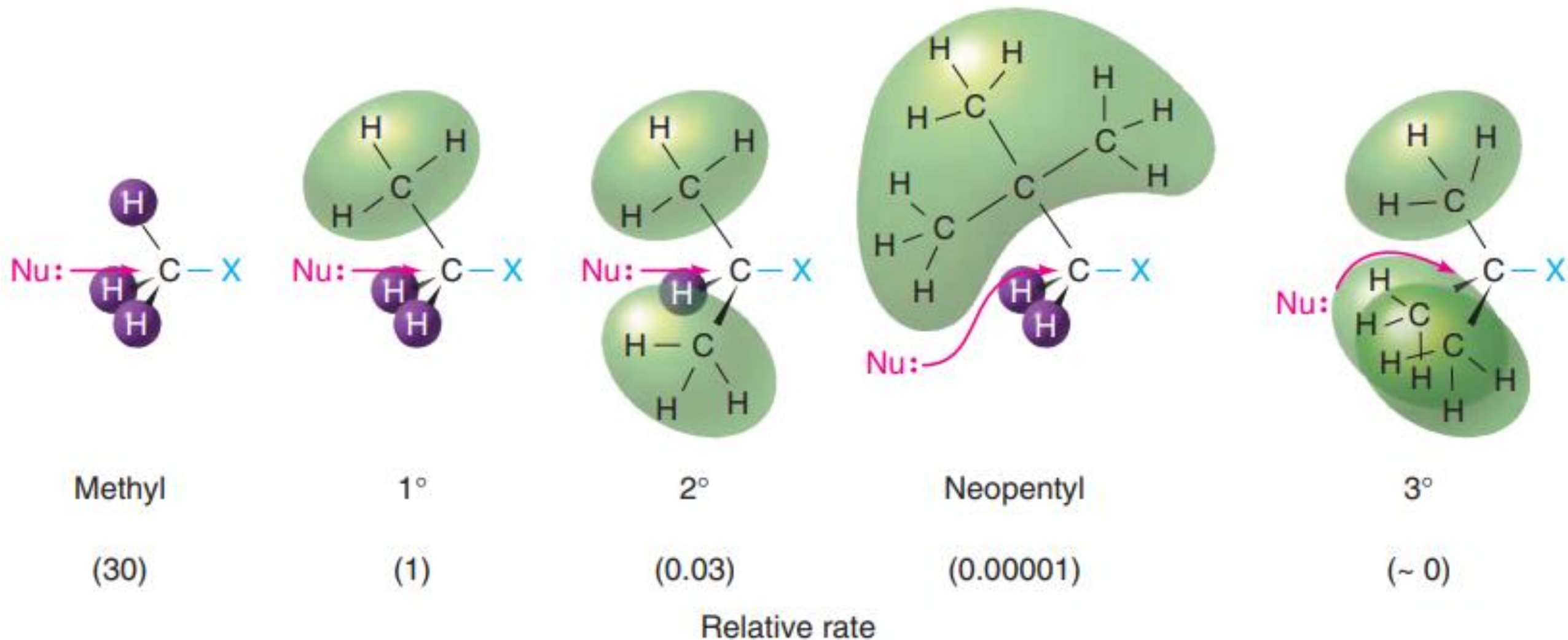
6.13A 1. The Effect of the Structure of the Substrate: S_N2 Reactions

TABLE 6.3 RELATIVE RATES OF REACTIONS OF ALKYL HALIDES IN S_N2 REACTIONS

Substituent	Compound	Approximate Relative Rate
Methyl	CH ₃ X	30
1°	CH ₃ CH ₂ X	1
2°	(CH ₃) ₂ CHX	0.03
Neopentyl	(CH ₃) ₃ CCH ₂ X	0.00001
3°	(CH ₃) ₃ CX	~0

Methyl > primary > secondary >> (tertiary—unreactive)


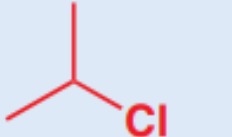
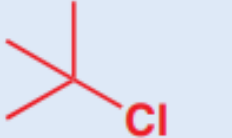


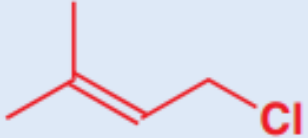

Steric effects and relative rates in the S_N2 reaction



- **A steric effect** is an effect on the relative rates caused by the space-filling properties of those parts of a molecule attached at or near the reacting site.
- **Steric hindrance** is when the spatial arrangement of atoms or groups at or near a reacting site of a molecule hinders or retards a reaction.

6.13A 1. The Effect of the Structure of the Substrate

Rates of solvolysis of alkyl chlorides in 50% aqueous ethanol at 44.6 °C

Compound	Relative rate	Comments
	0.07	primary chloride: probably all S _N 2
	0.12	secondary chloride: can do S _N 1 but not very well
	2100	tertiary chloride: very good at S _N 1
	1.0	primary but allylic: S _N 1 all right
	91	allylic cation is secondary at one end
	130000	allylic cation is tertiary at one end: compare with 2100 for simple tertiary
	7700	primary but allylic and benzylic

The table below shows the rates of solvolysis (i.e. a reaction in which the solvent acts as the nucleophile) in 50% aqueous ethanol for substituted allylic chlorides compared with benzylic chlorides and simple alkyl chlorides. The values give you an idea of the relative reactivity towards substitution of the different classes of compound. These rates are mostly S_N1, but there will be some S_N2 reactivity with the primary compounds.

The primary factor that determines the reactivity of organic substrates in an S_N1 reaction is the relative stability of the carbocation that is formed.

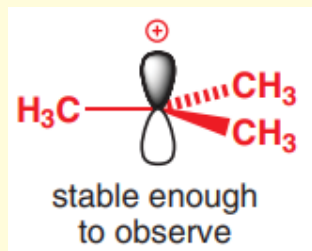
Stable carbocations as intermediates in S_N1 reactions

Type of cations

Example 1

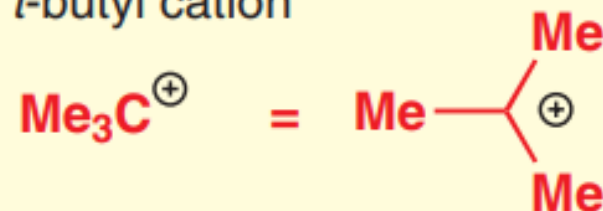
Example 2

simple alkyl



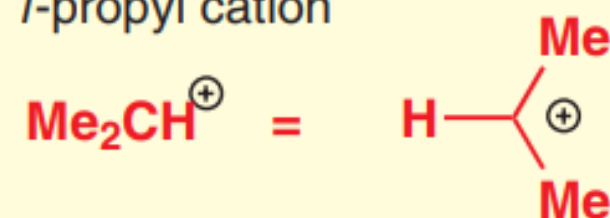
tertiary (good)

t-butyl cation



secondary (not so good)

i-propyl cation

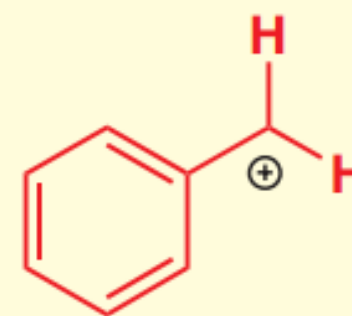


conjugated

allylic

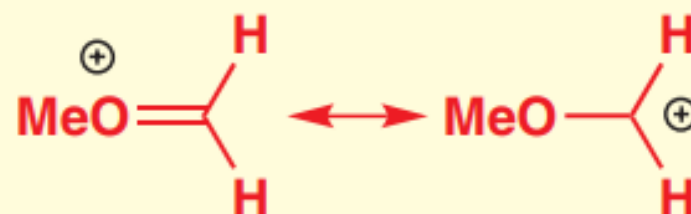


benzylic

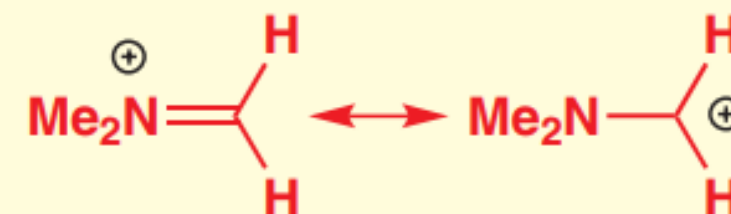


heteroatom-stabilized

oxygen-stabilized (oxonium ions)



nitrogen-stabilized (iminium ions)



6.13B The Effect of the Concentration and Strength of the Nucleophile

- The rate of an S_N1 reaction is unaffected by either the concentration or the identity of the nucleophile, because the nucleophile does not participate in the rate-determining step of an S_N1 reaction.
- The rate of an S_N2 reaction depends on both the concentration and the identity of the attacking nucleophile.
- The relative strengths of nucleophiles can be correlated with three structural features:

1. **A negatively charged nucleophile is always a more reactive nucleophile than its conjugate acid.** Thus HO^- is a better nucleophile than H_2O and RO^- is better than ROH .
2. **In a group of nucleophiles in which the nucleophilic atom is the same, nucleophilicities parallel basicities.** Oxygen compounds, for example, show the following order of reactivity:



This is also their order of basicity. An alkoxide ion (RO^-) is a slightly stronger base than a hydroxide ion (HO^-), a hydroxide ion is a much stronger base than a carboxylate ion (RCO_2^-), and so on.

3. **When the nucleophilic atoms are different, nucleophilicities may not parallel basicities.** For example, in protic solvents HS^- , $\text{N}\equiv\text{C}^-$, and I^- are all weaker bases than HO^- , yet they are **stronger nucleophiles** than HO^- .



- **Nucleophilicity versus Basicity**
While nucleophilicity and basicity are related, they are not measured in the same way.
- Basicity, as expressed by pK_a , is measured by the position of an equilibrium in an acid–base reaction.
- Nucleophilicity is measured by the relative rates of substitution reactions.

Effect of the Nucleophile on S_N2 reactions

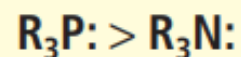
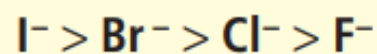
Relative rates (water = 1) of reaction with MeBr in EtOH

Nucleophile X ⁻	pK _a of HX	Relative rate
HO ⁻	15.7	1.2×10^4
PhO ⁻	10.0	2.0×10^3
AcO ⁻	4.8	9×10^2
H ₂ O	-1.7	1.0
ClO ₄ ⁻	-10	0

Relative rates (water = 1) of reaction with MeBr in EtOH

Nucleophile X ⁻	pK _a of HX	Relative rate
PhS ⁻	6.4	5.0×10^7
PhO ⁻	10.0	2.0×10^3

● Typically, nucleophilic power towards saturated carbon goes like this:



● Summary of the characteristics of the two types of nucleophile.

Hard nucleophiles X	Soft nucleophiles Y
small	large
charged	neutral
basic (HX weak acid)	not basic (HY strong acid)
low-energy HOMO	high-energy HOMO
like to attack C=O	like to attack saturated carbon
such as RO ⁻ , NH ₂ ⁻ , MeLi	such as RS ⁻ , I ⁻ , R ₃ P

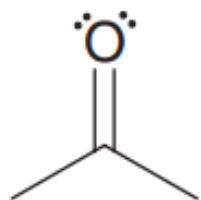
Nucleophiles in substitution reactions

Relative rates (water = 1) of reaction of nucleophiles with MeBr in EtOH

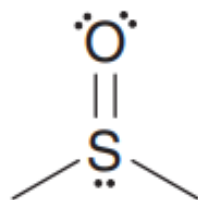
nucleophile	F ⁻	H ₂ O	Cl ⁻	Et ₃ N	Br ⁻	PhO ⁻	EtO ⁻	I ⁻	PhS ⁻
relative rate	0.0	1.0	1100	1400	5000	2.0×10^3	6×10^4	1.2×10^5	5.0×10^7

6.13C Solvent Effects in S_N2 and S_N1 Reactions

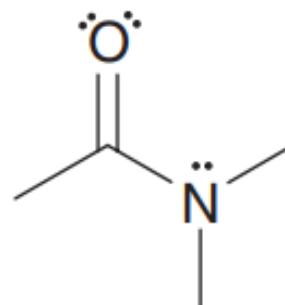
- S_N2 reactions are favored by **polar aprotic solvents** (e.g., acetone, DMF, DMSO).
 - S_N1 reactions are favored by **polar protic solvents** (e.g., EtOH, MeOH, H₂O).
- ❑ **Important reasons for these solvent effects have to do with**
- (a) minimizing the solvent's interaction with the nucleophile in S_N2 reactions, and
 - (b) facilitating ionization of the leaving group and stabilizing ionic intermediates by solvents in S_N1 reactions.
- ❑ **Polar Aprotic Solvents Favor S_N2 Reactions**
- ❑ An aprotic solvent does not have hydrogen atoms that are capable of hydrogen bonding.
 - ❑ Polar, aprotic solvents such as acetone, DMF, DMSO, and HMPA are often used alone or as co-solvents for S_N2 reactions.



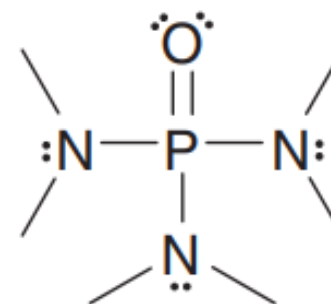
Acetone



DMSO
(Dimethylsulfoxide)

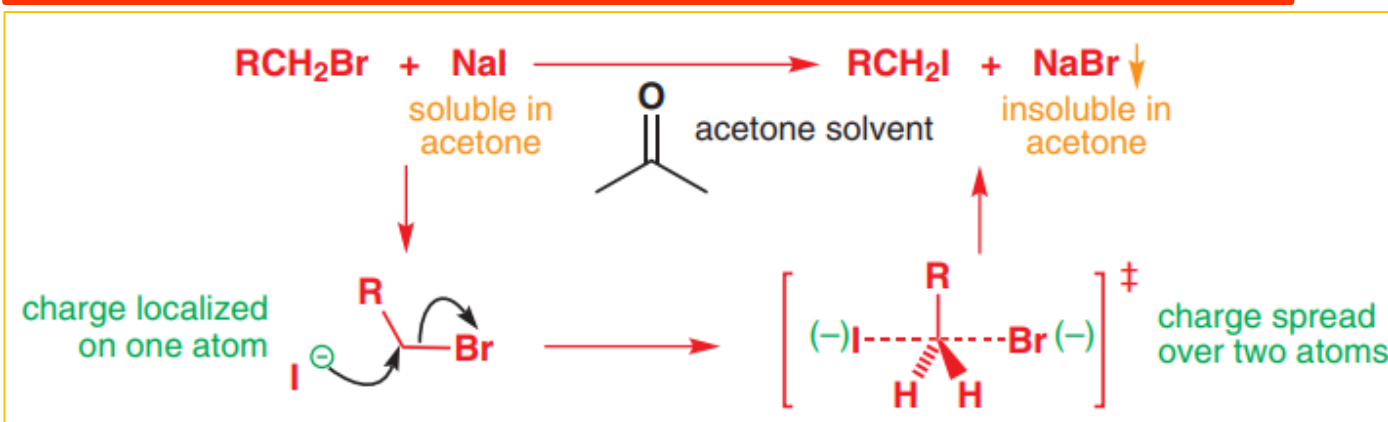
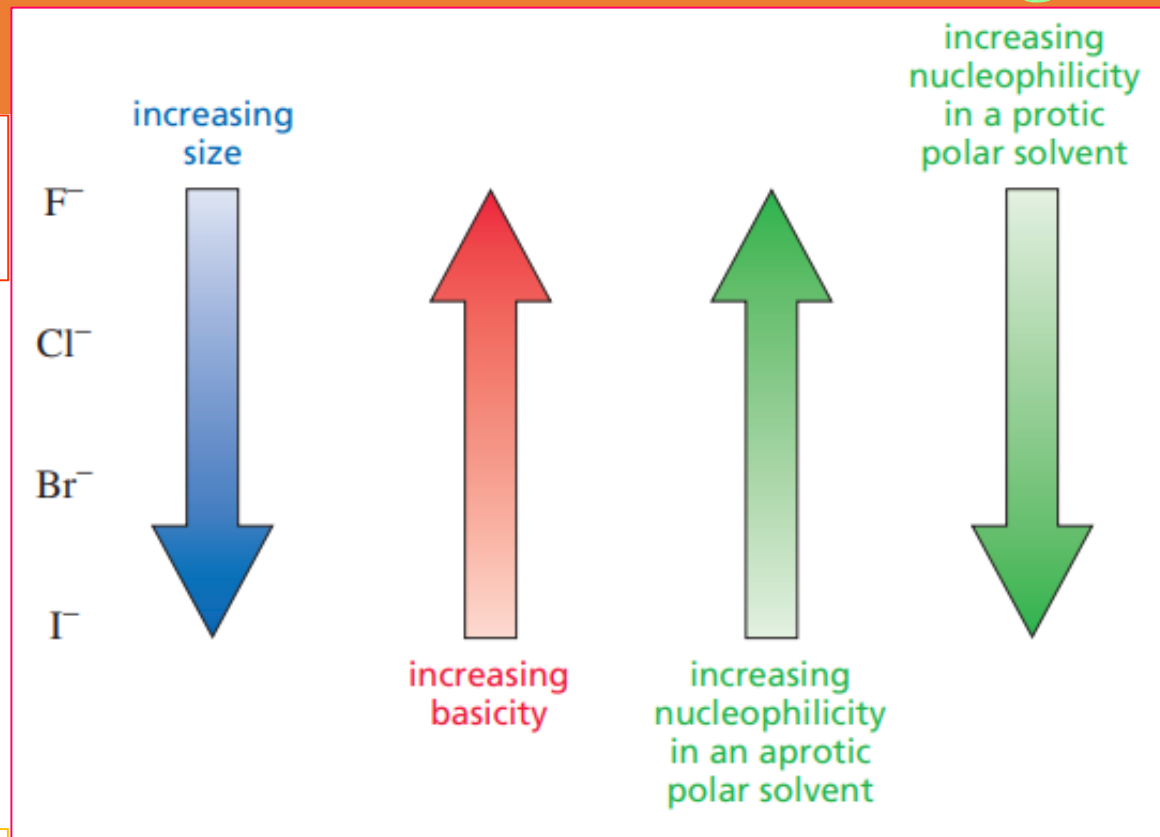
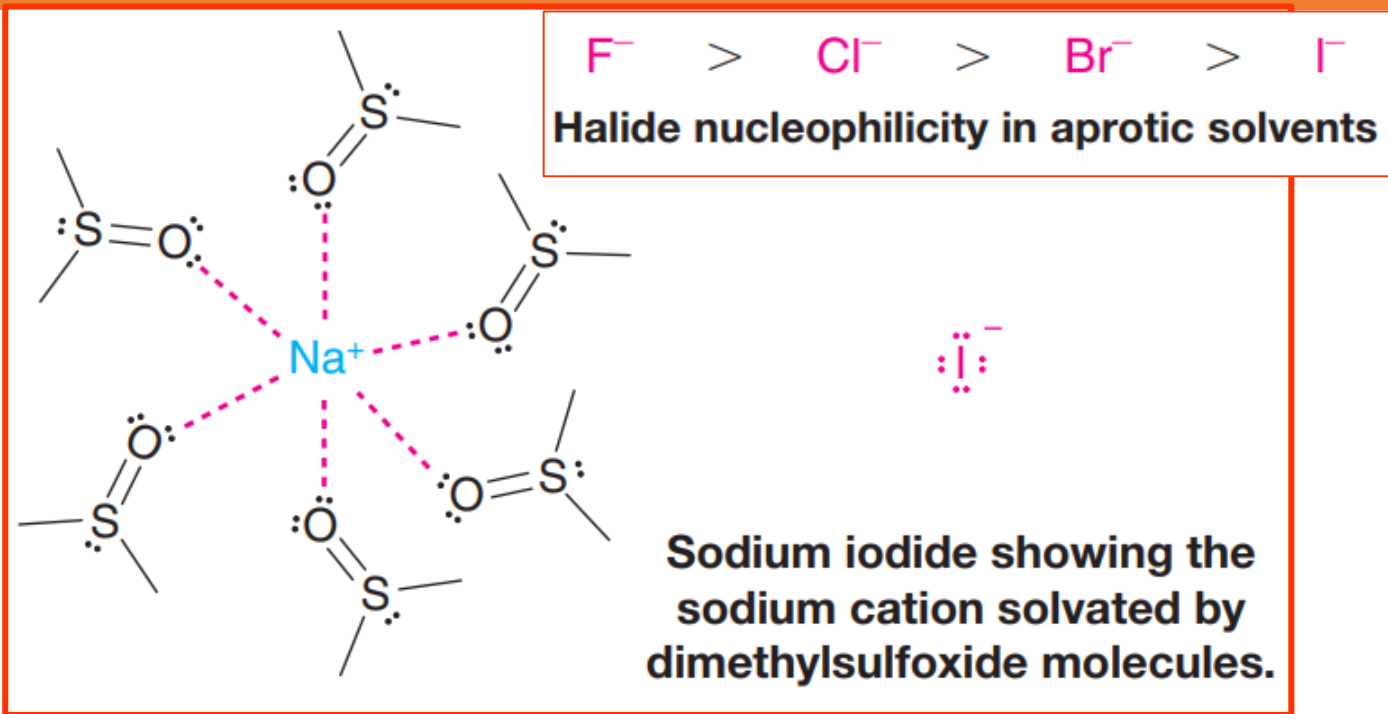


DMF
(*N,N*-Dimethyl-
formamide)



HMPA
(Hexamethyl
phosphoramide)

The rates of S_N2 reactions generally are vastly increased when they are carried out in polar aprotic solvents. The increase in rate can be as large as a million fold.



Acetone also assists this reaction because it dissolves sodium iodide but not the sodium bromide product, which precipitates from solution and prevents bromide acting as a competing nucleophile.

Beauty of Solvents in a reaction

Polar Protic Solvents Favor S_N1 Reactions

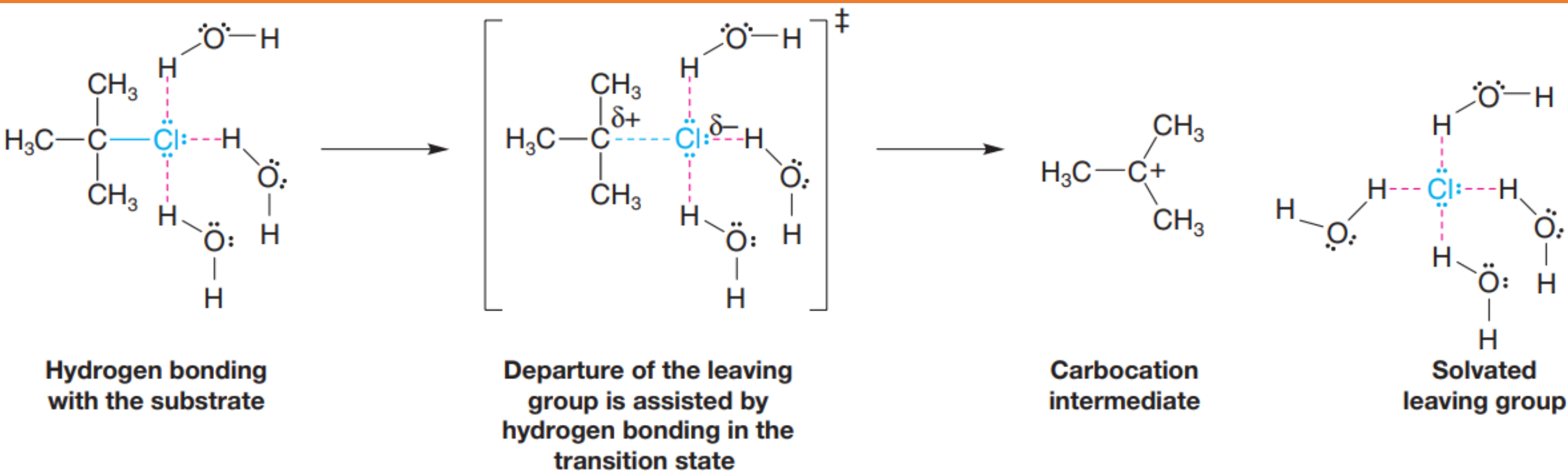
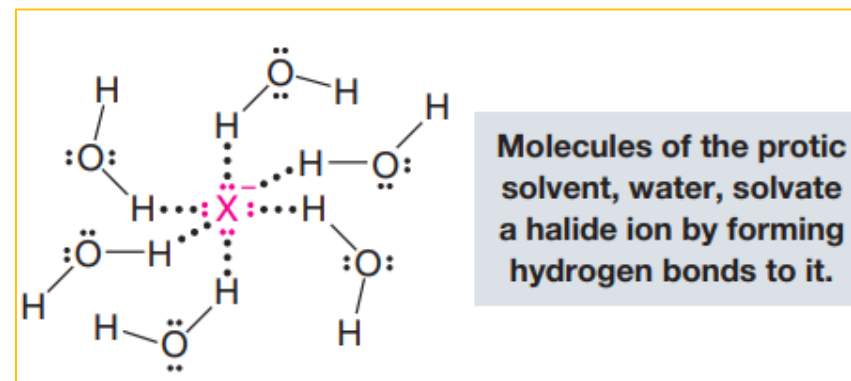


TABLE 6.4 DIELECTRIC CONSTANTS OF COMMON SOLVENTS

	Solvent	Formula	Dielectric Constant
↑ Increasing solvent polarity ↓	Water	H ₂ O	80
	Formic acid	HCO ₂ H	59
	Dimethyl sulfoxide (DMSO)	CH ₃ SOCH ₃	49
	<i>N,N</i> -Dimethylformamide (DMF)	HCON(CH ₃) ₂	37
	Acetonitrile	CH ₃ C≡N	36
	Methanol	CH ₃ OH	33
	Hexamethylphosphoramide (HMPA)	[(CH ₃) ₂ N] ₃ P=O	30
	Ethanol	CH ₃ CH ₂ OH	24
	Acetone	CH ₃ COCH ₃	21
	Acetic acid	CH ₃ CO ₂ H	6

However, Protic Solvents Hinder the Nucleophile in S_N2 Reactions



Halide nucleophilicity in protic solvents

✖✖✖ The extent of hydrogen bonding with the nucleophile varies with the identity of the nucleophile. Hydrogen bonding with a small nucleophilic atom is stronger than to a larger nucleophilic atom among elements in the same group (column) of the periodic table.

✖✖✖ *For example, fluoride anion is more strongly solvated than the other halides because it is the smallest halide anion and its charge is the most concentrated. Hence, in a protic solvent fluoride is not as effective a nucleophile as the other halide anions. Iodide is the largest halide anion and it is the most weakly solvated in a protic solvent; hence, it is the strongest nucleophile among the halide anions.*

- In a protic solvent, the general trend in *nucleophilicity* among the halide anions is as follows:



Halide nucleophilicity in protic solvents

The same effect holds true when we compare sulfur nucleophiles with oxygen nucleophiles. ***Sulfur atoms are larger than oxygen atoms and hence they are not solvated as strongly in a protic solvent.*** Thus, thiols (R-SH) are stronger nucleophiles than alcohols, and RS⁻ anions are better nucleophiles than RO⁻ anions.

Polarizability vs Nucleophilicity

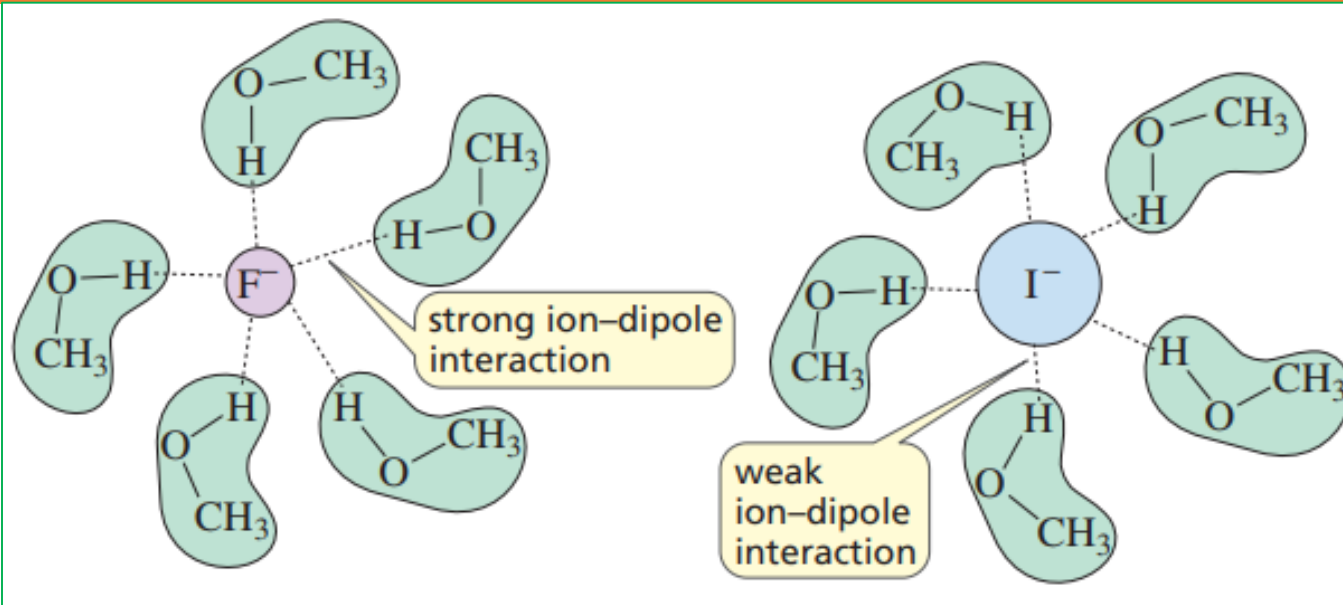
- ✦ The greater reactivity of nucleophiles with large nucleophilic atoms is not entirely related to solvation.
- ✦ Larger atoms have greater polarizability (their electron clouds are more easily distorted); therefore, a larger nucleophilic atom can donate a greater degree of electron density to the substrate than a smaller nucleophile whose electrons are more tightly held.

The relative nucleophilicities of some common nucleophiles in protic solvents are as follows:



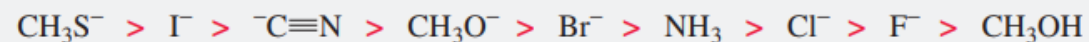
Relative nucleophilicity in protic solvents

Why Is the Nucleophilicity Affected by the Solvent?

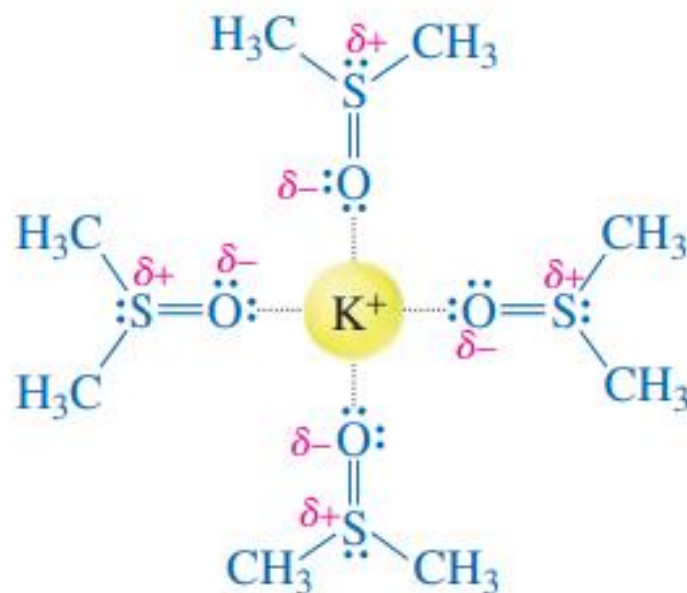
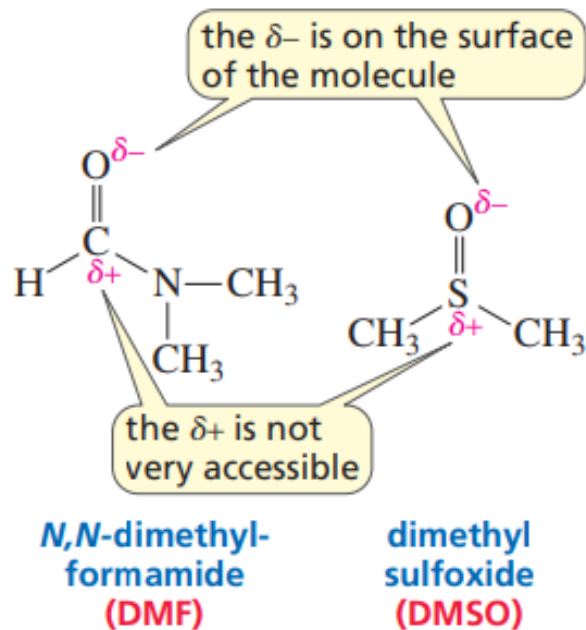
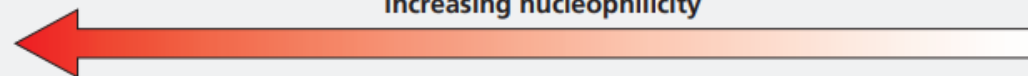


It is easier, therefore, to break the ion–dipole interactions between an **iodide ion (a weak base)** and the solvent than between a **fluoride ion (a stronger base)** and the solvent. In a protic solvent, therefore, an iodide ion, even though it is a weaker base, is a better nucleophile than a fluoride ion.

Relative Nucleophilicity toward CH_3I in Methanol



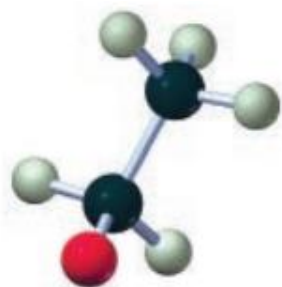
increasing nucleophilicity



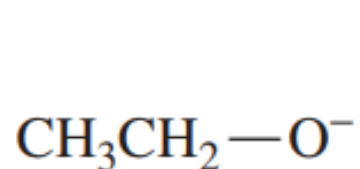
Fluoride ion would be an even better nucleophile in a nonpolar solvent (such as hexane) because there would not be any ion–dipole interactions between the ion and the nonpolar solvent. Ionic compounds, however, are insoluble in nonpolar solvents, but they dissolve in aprotic polar solvents. Fluoride ion is also a good nucleophile in the gas phase, where there are no solvent molecules.

Nucleophilicity Is Affected by Steric Effect

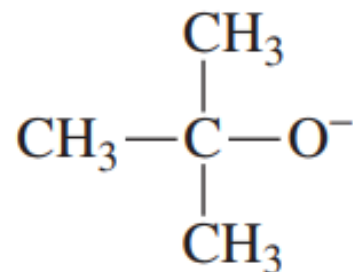
Nucleophilicity is *affected* by steric effects because a bulky nucleophile cannot approach the back side of a carbon as easily as a less sterically hindered nucleophile can. Basicity, on the other hand, is relatively *unaffected* by steric effects because a base removes an unhindered proton.



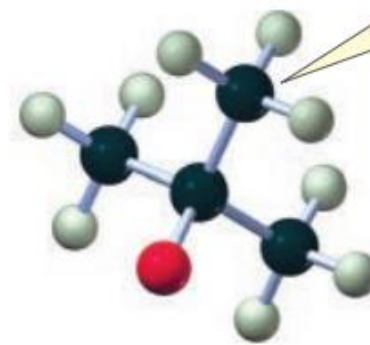
ethoxide ion



ethoxide ion
better nucleophile



tert-butoxide ion
stronger base

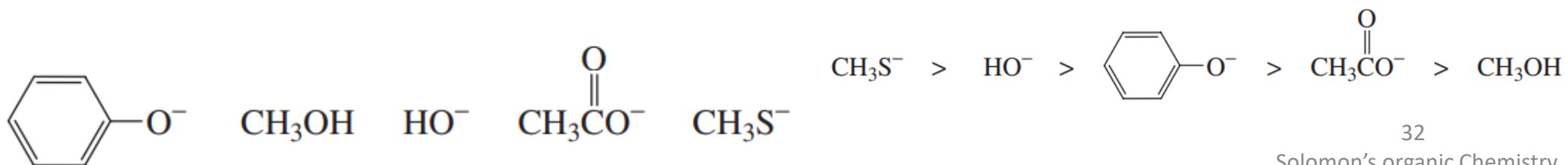


tert-butoxide ion

the 3 methyl groups make it difficult for the oxygen to approach the back side of a carbon

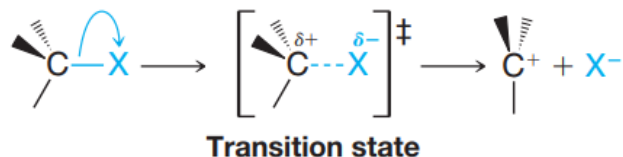
Therefore, *tert*-butoxide ion, with its three methyl groups, is a poorer nucleophile than ethoxide ion, even though *tert*-butoxide ion is a stronger base ($\text{p}K_a$ of *tert*-butanol = 18) than ethoxide ion ($\text{p}K_a$ of ethanol = 16).

Rank the following species from best nucleophile to poorest nucleophile in an aqueous solution:



6.13D The Nature of the Leaving Group

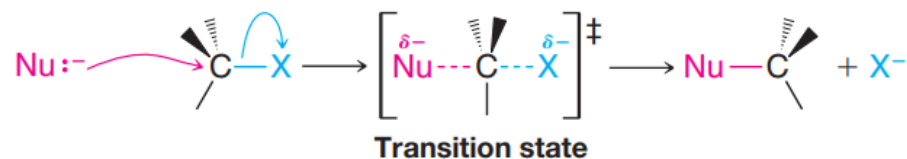
S_N1 Reaction (Rate-Limiting Step)



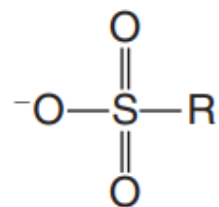
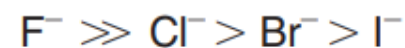
Among the halogens, an iodide ion is the best leaving group and a fluoride ion is the poorest:



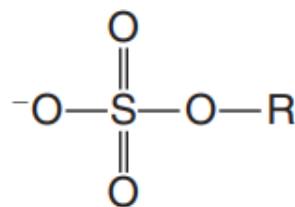
S_N2 Reaction



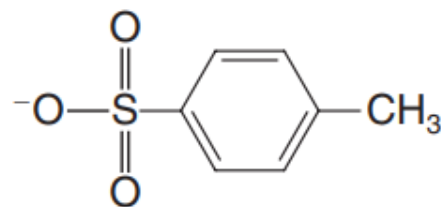
The order is the opposite of the basicity in an aprotic solvent:



An alkane sulfonate ion



An alkyl sulfate ion

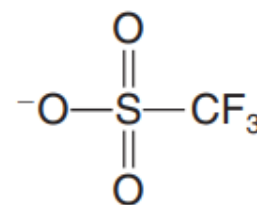


p-Toluenesulfonate ion

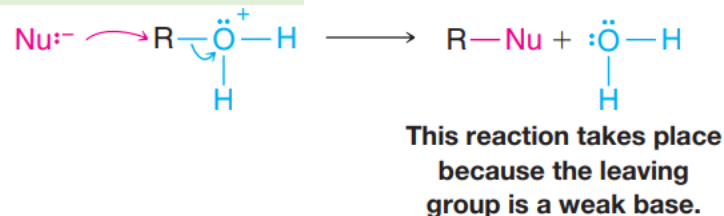
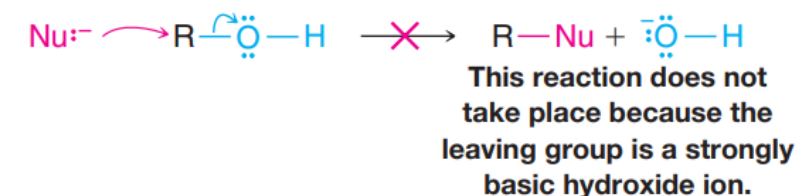
Other weak bases that are good leaving groups, are alkane sulfonate ions, alkyl sulfate ions, and the *p*-toluenesulfonate ion:

These anions are all the conjugate bases of very strong acids.

The trifluoromethanesulfonate ion (CF_3SO_3^- , commonly called the triflate ion) is one of the best leaving groups known to chemists. It is the conjugate base of $\text{CF}_3\text{SO}_3\text{H}$, an exceedingly strong acid ($\text{pK}_a \sim -5$ to -6):

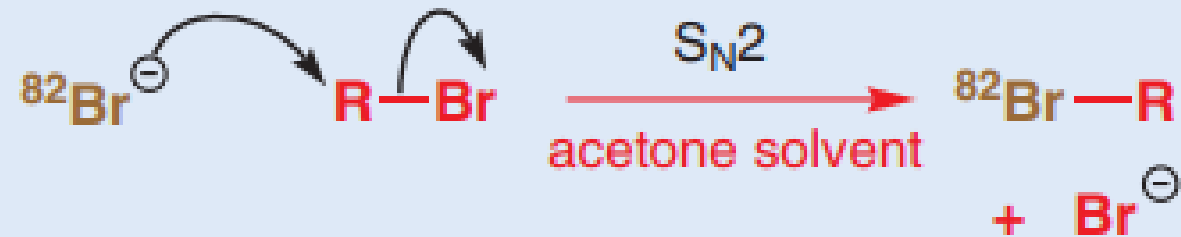


Triflate ion
(a “super” leaving group)

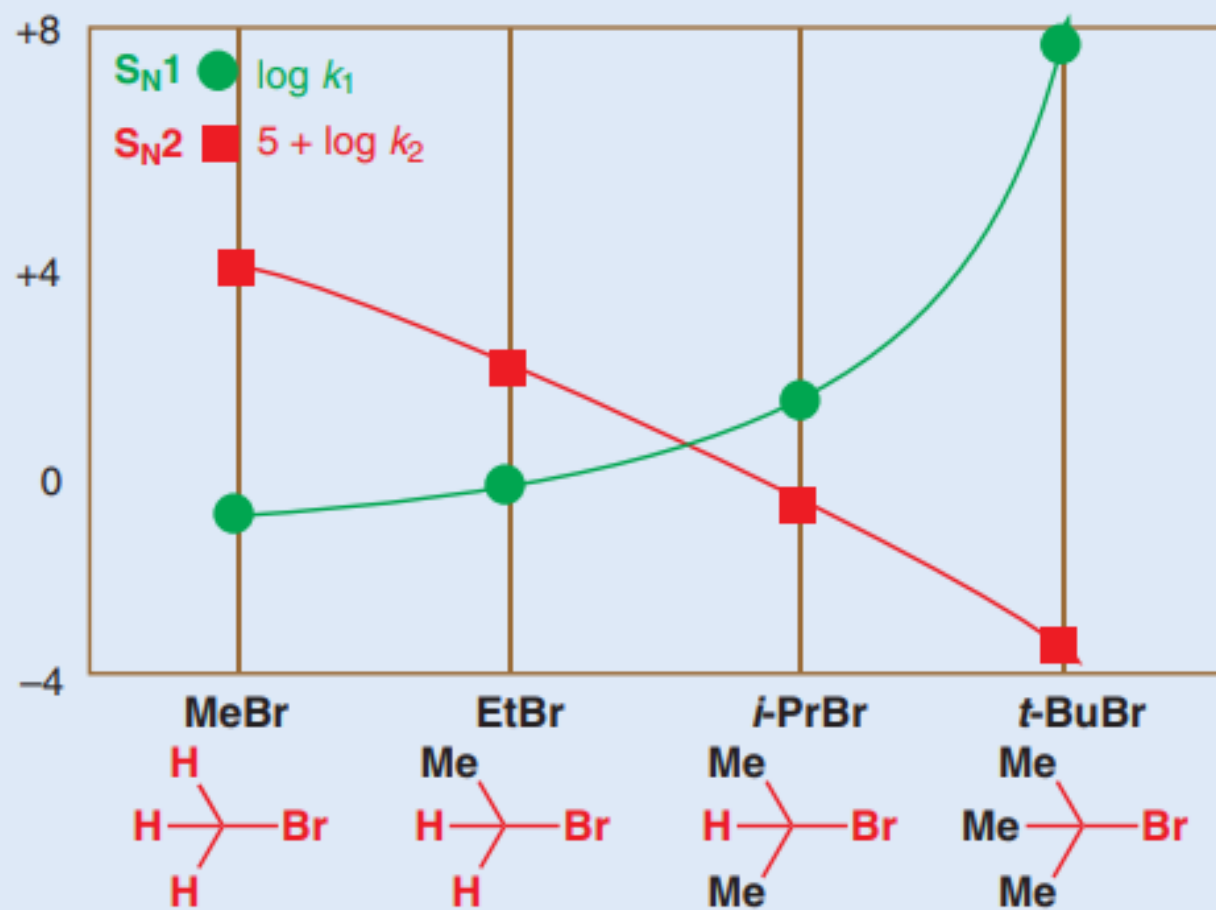


Strongly basic ions rarely act as leaving groups.

Quantifying the rates of S_N1 and S_N2 reactions

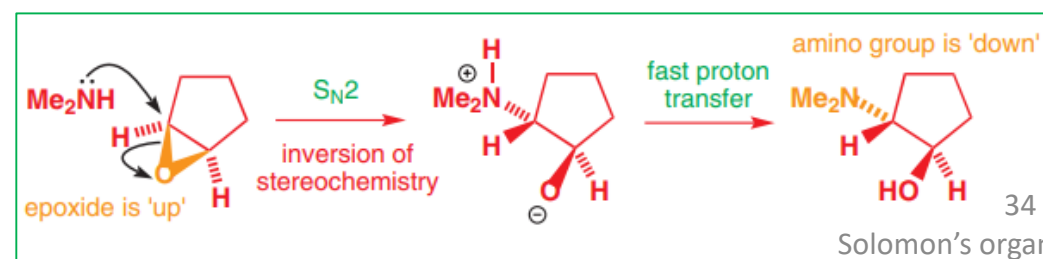
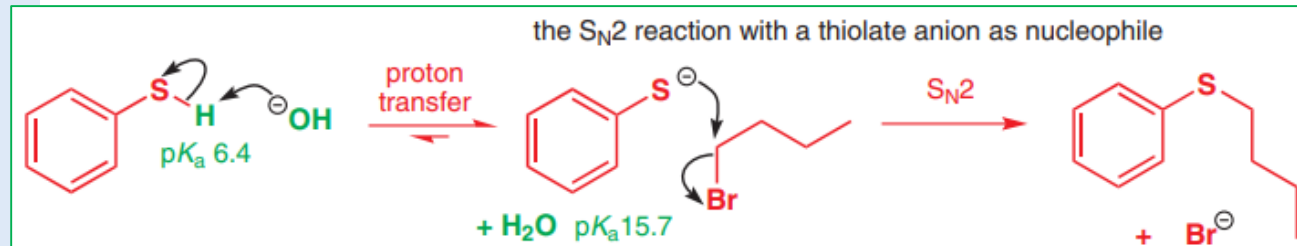


Rates of S_N1 and S_N2 rates for simple alkyl bromides

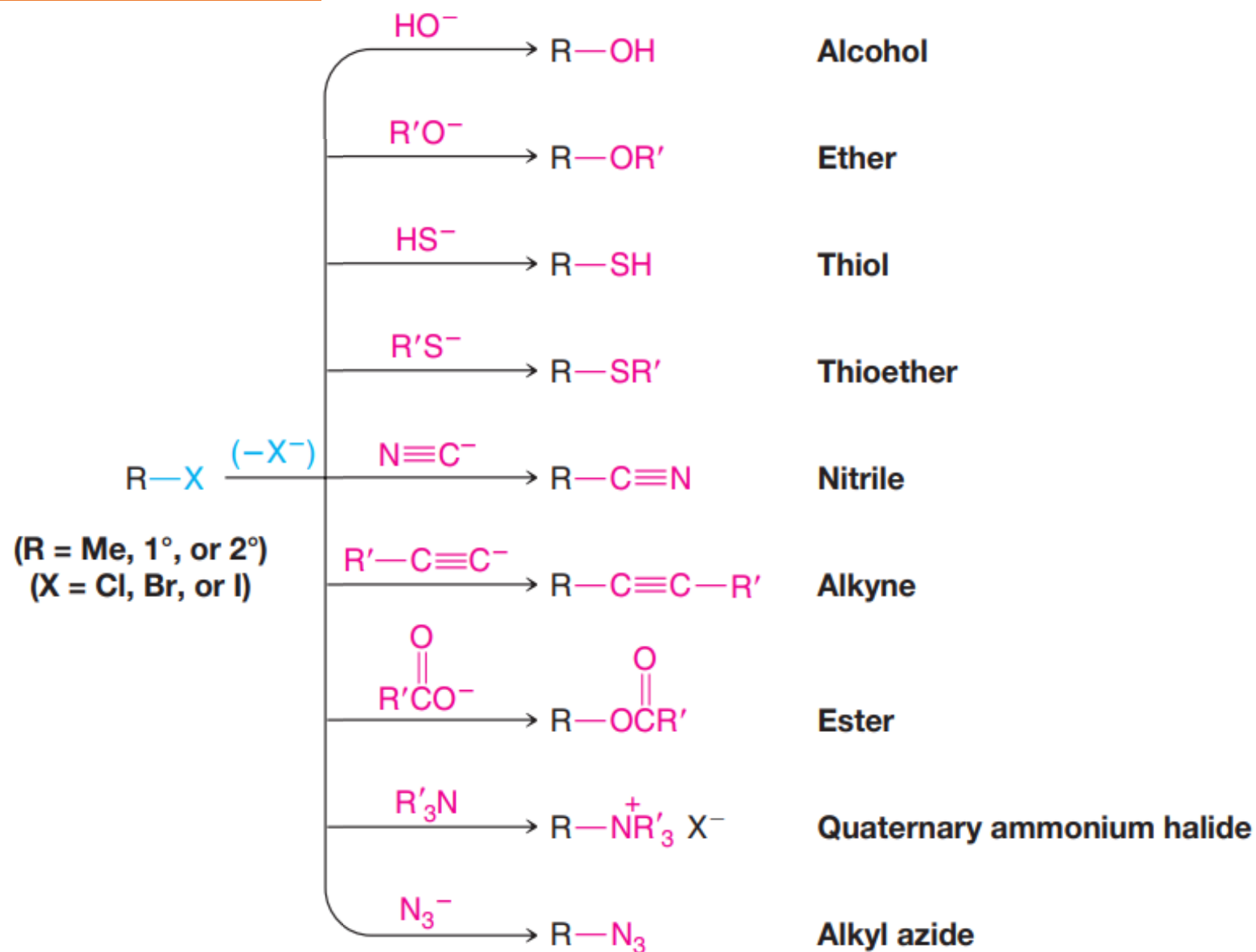


Rates of S_N1 and S_N2 reactions of simple alkyl bromides

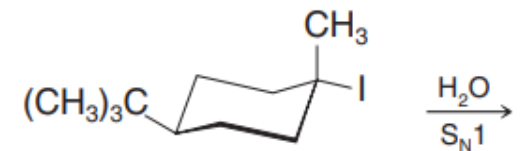
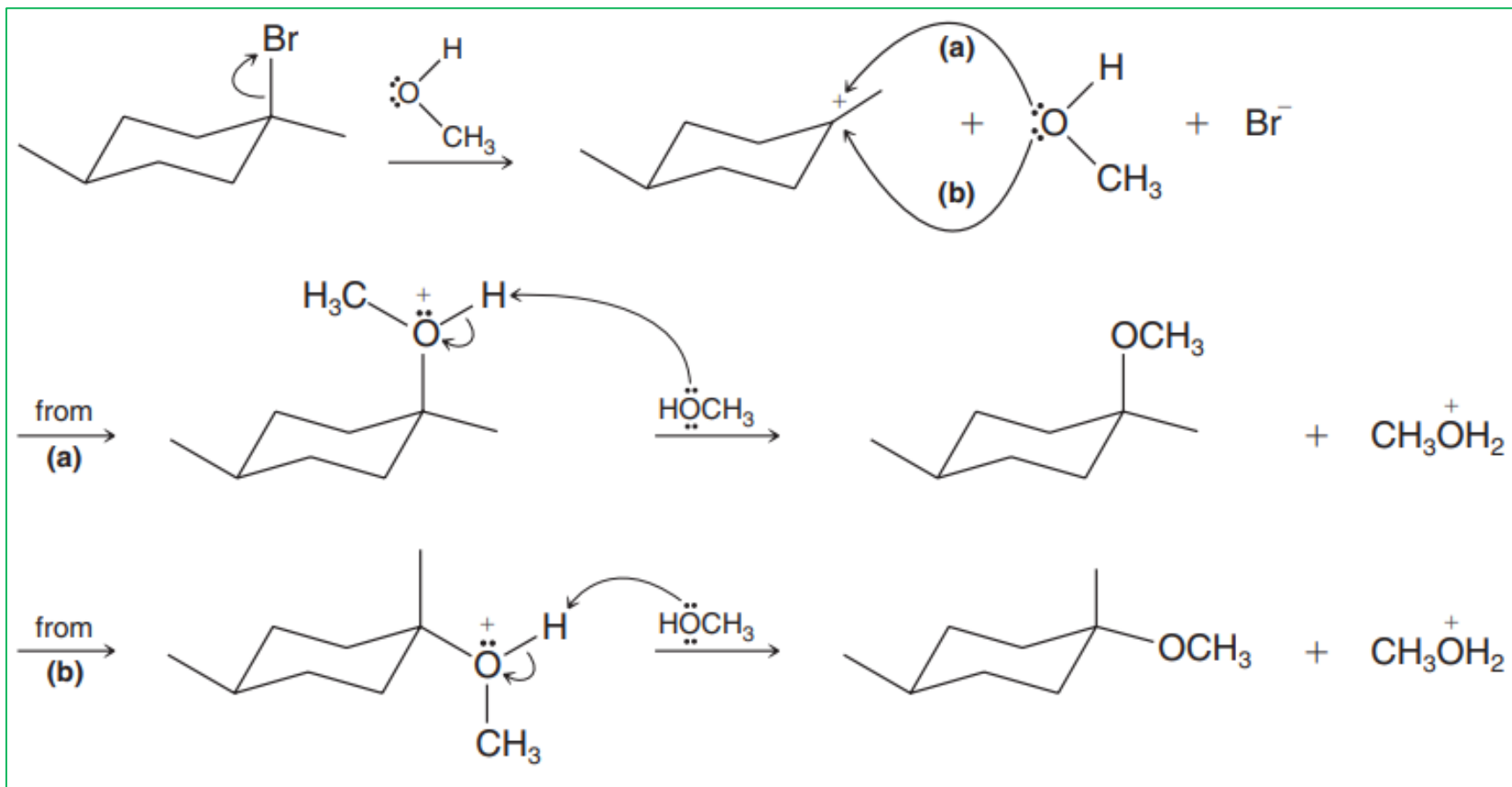
alkyl bromide type	CH ₃ Br methyl	CH ₃ CH ₂ Br primary	(CH ₃) ₂ CHBr secondary	(CH ₃) ₃ CBr tertiary
k_1 (s ⁻¹)	0.6	1.0	26	10 ⁸
10 ⁵ k_2 (M ⁻¹ dm ⁻³ s ⁻¹)	13,000	170	6	0.0003
relative k_1	2 × 10 ⁻²	4 × 10 ⁻²	1	4 × 10 ⁶
relative k_2	6 × 10 ³	30	1	5 × 10 ⁻⁵



6.14 Organic Synthesis: Functional Group Transformations Using S_N2 Reaction



Keeping in mind that carbocations have a trigonal planar structure, (a) write a structure for the carbocation intermediate and (b) write structures for the alcohol (or alcohols) that you would expect from reaction of iodocyclohexane shown on the right side in water:



Can you all try this?