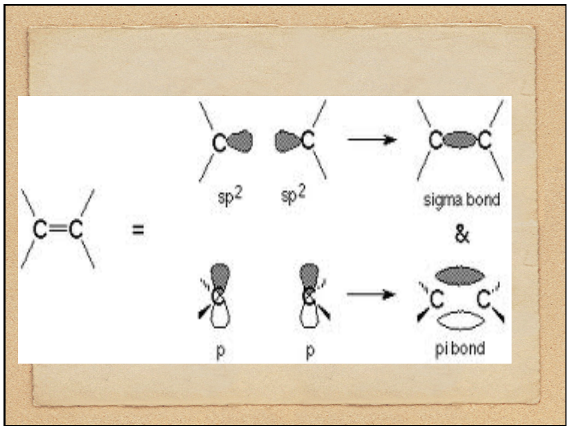
Chapter 3

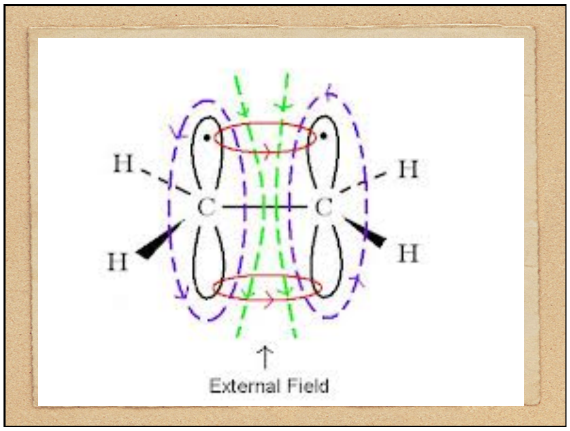
Alkenes

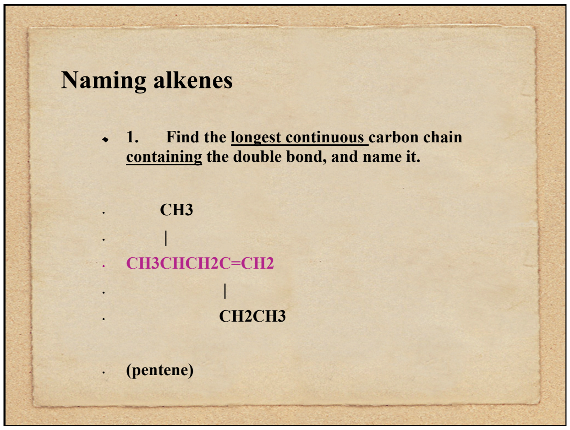
- **EQ: How do I name and draw the molecular structural and skeletal structure for alkenes?**

Alkenes

- Definition: Compounds containing C=C
- Example: CH2=CH2





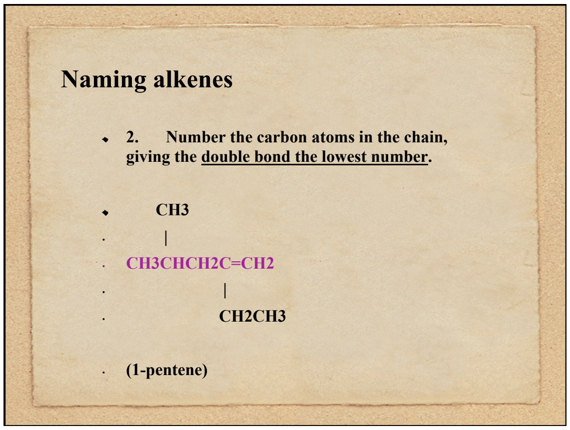


Naming alkenes

- 1. Find the <u>longest continuous</u> carbon chain <u>containing</u> the double bond, and name it.

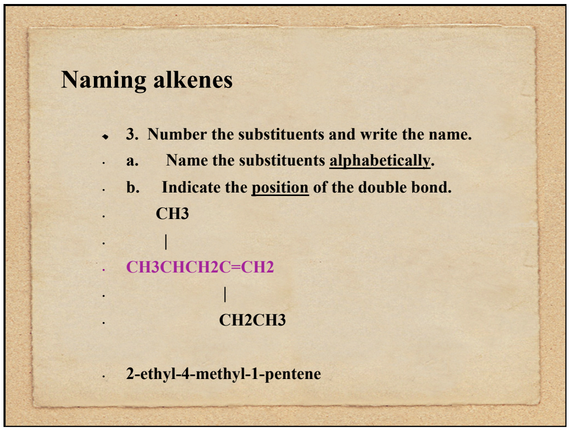
CH3
|
CH3CHCH2C=CH2
|
CH2CH3

(pentene)



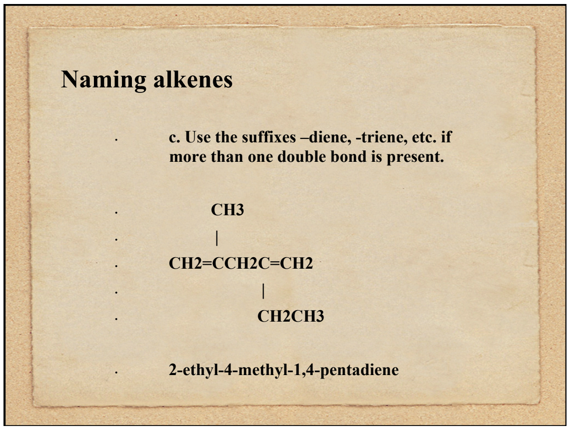
Naming alkenes

- 2. Number the carbon atoms in the chain, giving the <u>double bond the lowest number</u>.
- CH3
- |
- CH3CHCH2C=CH2
- |
- CH2CH3
- (1-pentene)



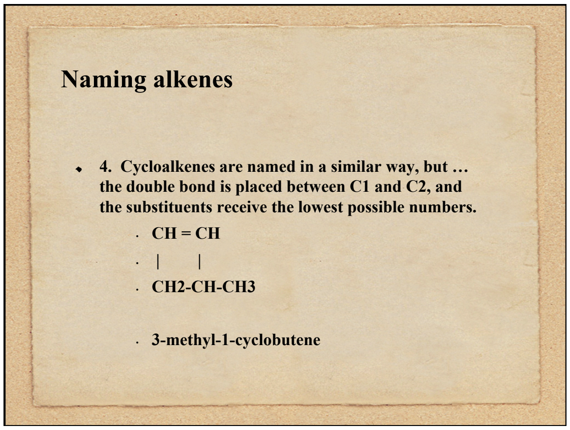
Naming alkenes

- 3. Number the substituents and write the name.
- a. Name the substituents <u>alphabetically</u>.
- b. Indicate the <u>position</u> of the double bond.
- CH3
- |
- CH3CHCH2C=CH2
- |
- CH2CH3
- 2-ethyl-4-methyl-1-pentene



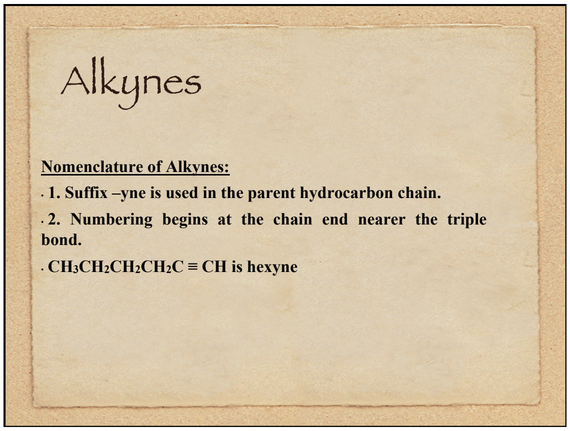
Naming alkenes

- c. Use the suffixes –diene, -triene, etc. if more than one double bond is present.
- CH3
- |
- CH2=CCH2C=CH2
- |
- CH2CH3
- 2-ethyl-4-methyl-1,4-pentadiene



Naming alkenes

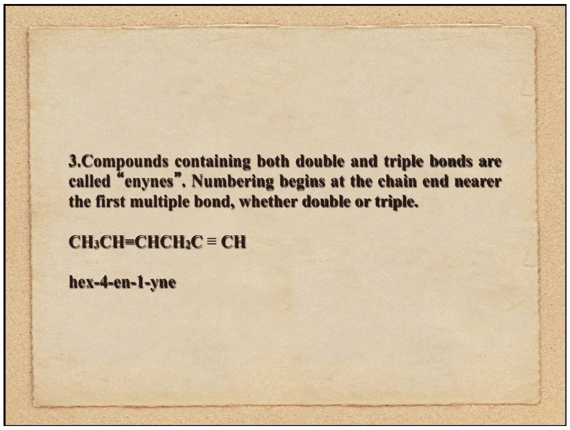
- 4. Cycloalkenes are named in a similar way, but … the double bond is placed between C1 and C2, and the substituents receive the lowest possible numbers.
  - CH = CH
  - | |
  - CH2-CH-CH3
  - 3-methyl-1-cyclobutene



Alkynes

Nomenclature of Alkynes:

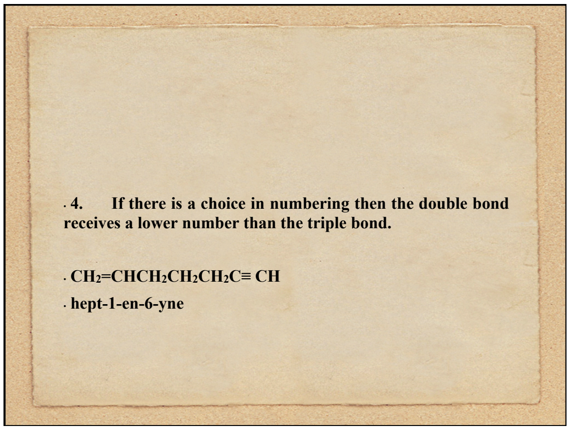
- 1. Suffix –yne is used in the parent hydrocarbon chain.
- 2. Numbering begins at the chain end nearer the triple bond.
- $CH_3CH_2CH_2CH_2C \equiv CH$ is hexyne



3.Compounds containing both double and triple bonds are called “enynes”. Numbering begins at the chain end nearer the first multiple bond, whether double or triple.

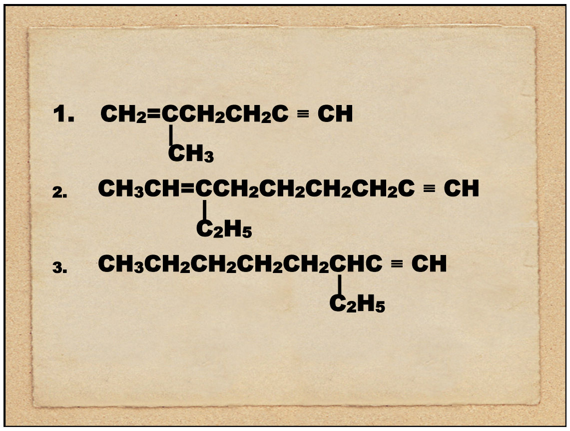
$CH_3CH{=}CHCH_2C \equiv CH$

hex-4-en-1-yne

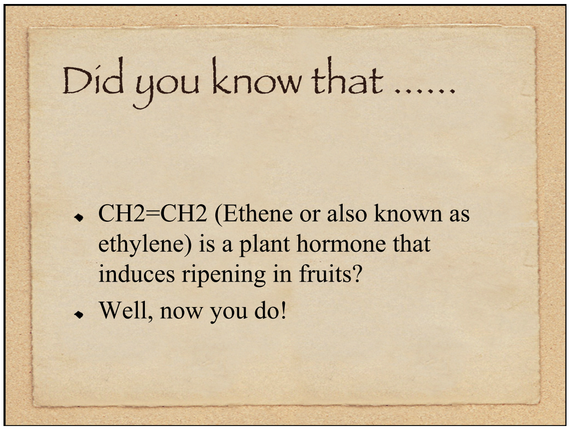


- 4. If there is a choice in numbering then the double bond receives a lower number than the triple bond.

- $CH_2{=}CHCH_2CH_2CH_2C{\equiv}\,CH$
- hept-1-en-6-yne

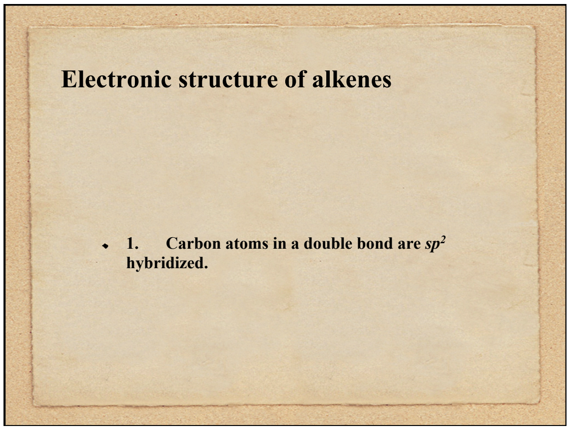


1. $CH_2{=}\underset{\displaystyle CH_3}{\underset{|}{C}}CH_2CH_2C \equiv CH$
2. $CH_3CH{=}\underset{\displaystyle C_2H_5}{\underset{|}{C}}CH_2CH_2CH_2CH_2C \equiv CH$
3. $CH_3CH_2CH_2CH_2CH_2\underset{\displaystyle C_2H_5}{\underset{|}{C}}HC \equiv CH$



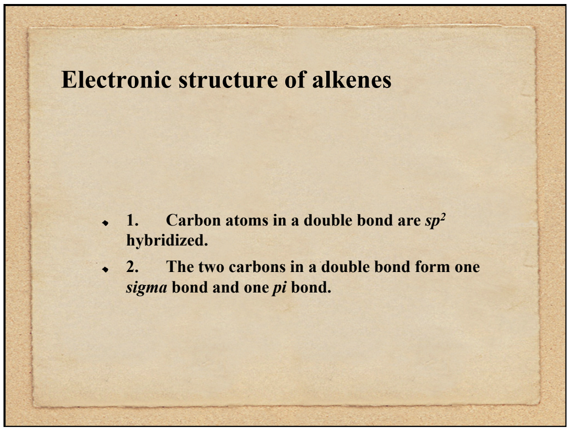
Did you know that ……

- CH2=CH2 (Ethene or also known as ethylene) is a plant hormone that induces ripening in fruits?
- Well, now you do!



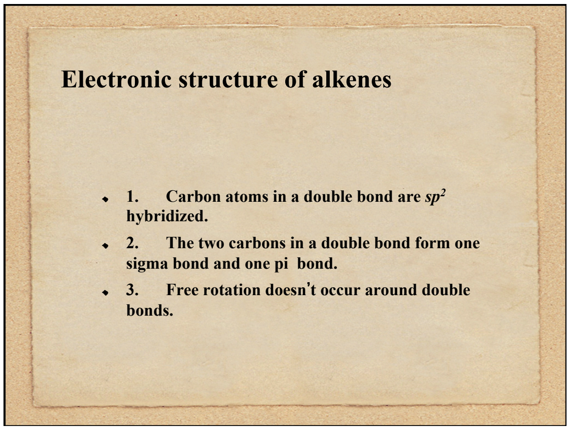
Electronic structure of alkenes

- 1. Carbon atoms in a double bond are sp^2 hybridized.



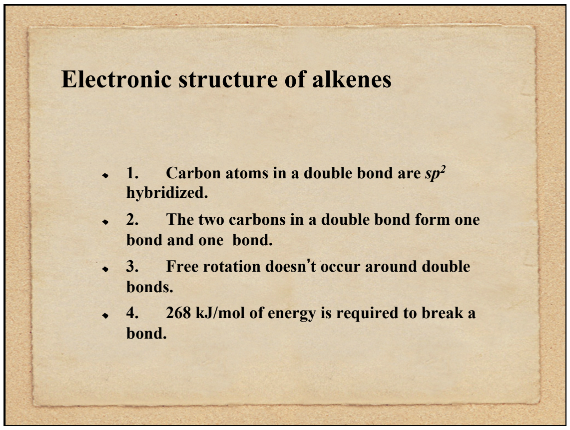
Electronic structure of alkenes

- 1. Carbon atoms in a double bond are sp^2 hybridized.
- 2. The two carbons in a double bond form one *sigma* bond and one *pi* bond.



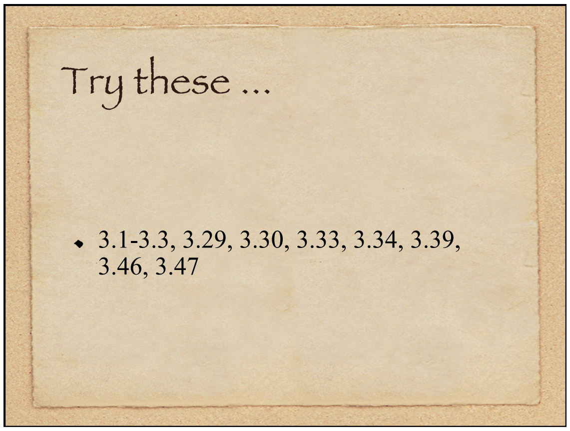
Electronic structure of alkenes

- 1. Carbon atoms in a double bond are sp^2 hybridized.
- 2. The two carbons in a double bond form one sigma bond and one pi bond.
- 3. Free rotation doesn't occur around double bonds.



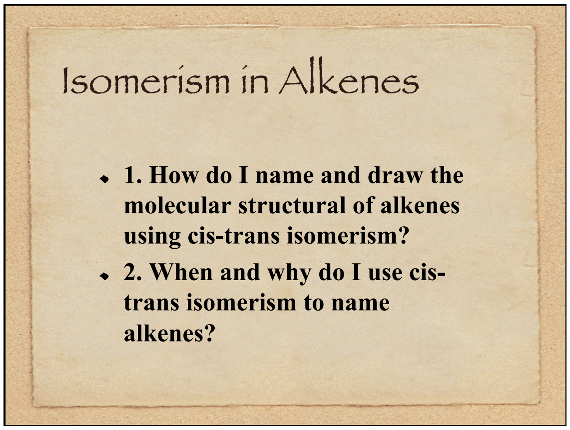
Electronic structure of alkenes

- 1. Carbon atoms in a double bond are *sp*^{2} hybridized.
- 2. The two carbons in a double bond form one bond and one bond.
- 3. Free rotation doesn't occur around double bonds.
- 4. 268 kJ/mol of energy is required to break a bond.



Try these …

- 3.1-3.3, 3.29, 3.30, 3.33, 3.34, 3.39, 3.46, 3.47



Isomerism in Alkenes

- **1. How do I name and draw the molecular structural of alkenes using cis-trans isomerism?**
- **2. When and why do I use cis-trans isomerism to name alkenes?**

- Draw and show me the structures of the following…(Use model kits)
- a. 1, 2-dichloroethene
- b. 1, 1-dichloroethene

Cis-trans isomerism

- **a. A *di*substituted alkene can have substituents either on the same side of the double bond (cis) or on opposite sides (trans).**
- **b. These isomers don't interconvert because free rotation about a double bond isn't possible.**
- **c. Cis-trans isomerism doesn't occur if one carbon in the double bond is bonded to identical substituents.**
- **d. Cis alkenes are less stable than their trans isomers. (Why is that so?)**

Bow-Tie structures

- **Use bow-tie structures to draw di, tri and tetra substituted alkenes.**

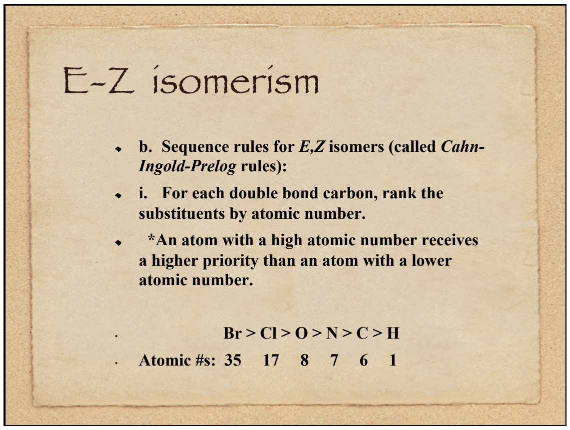
Try these …

- 3.4, 3.5, 3.35, 3.37, 3.38

- **1. How do I name and draw the molecular structural of alkenes using E,Z designation?**
- **2. When and why do I use E,Z designation to name alkenes?**

E-Z isomerism

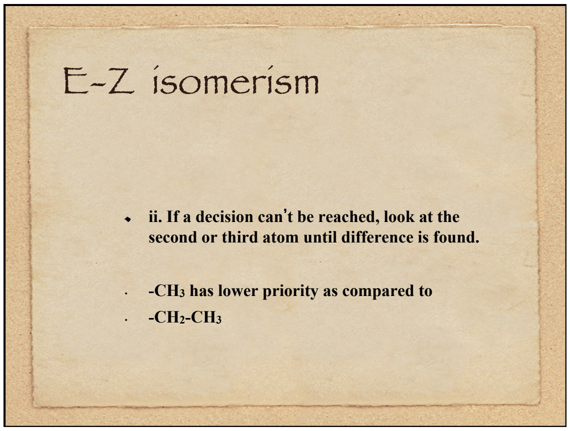
- **a. The *E,Z* system is used to describe the arrangement of substituents around a double bond that can't be described by the cis-trans system.**
- **It is used when there are more than 2 substituents.**



E-Z isomerism

- b. Sequence rules for ***E,Z*** isomers (called ***Cahn-Ingold-Prelog*** rules):
- i. For each double bond carbon, rank the substituents by atomic number.
- *An atom with a high atomic number receives a higher priority than an atom with a lower atomic number.

	Br >	Cl >	O >	N >	C >	H
Atomic #s:	35	17	8	7	6	1

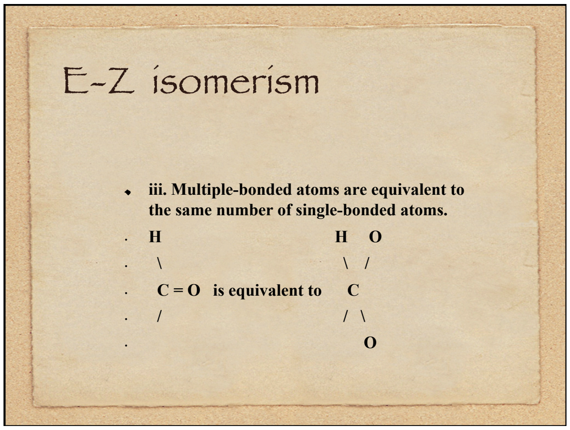


E-Z isomerism

- ii. If a decision can't be reached, look at the second or third atom until difference is found.

$-CH_3$ has lower priority as compared to

$-CH_2-CH_3$



E-Z isomerism

- iii. Multiple-bonded atoms are equivalent to the same number of single-bonded atoms.

```
H                         H   O
  \                         \  /
  C = O   is equivalent to   C
  /                         /  \
                                O
```

E-Z isomerism

- c. In a *Z* isomer, the two groups of higher priority are on the *same (Z-zame :-)* side of the alkene double bond.
- d. In an *E* isomer, the two groups of higher priority are on *opposite* sides of the alkene double bond.

Try these ...

- 3.6-3.9, 3.19- 3.20, 3.31, 3.32, 3.36, 3.41, 3.42, 3.43, 3.45, 3.48, 3.49

Organic Reactions

- **E.Q.What are the 4 kinds of organic reactions? Explain each one with the help of an example.**

A. Kinds Of Organic Reactions

- 1. **Addition** reactions occur when two reactants add to form one product, with no atoms left over.

$CH_2 = CH_2 + HCl \rightarrow CH_3 - CH_2Cl$

Kinds Of Organic Reactions

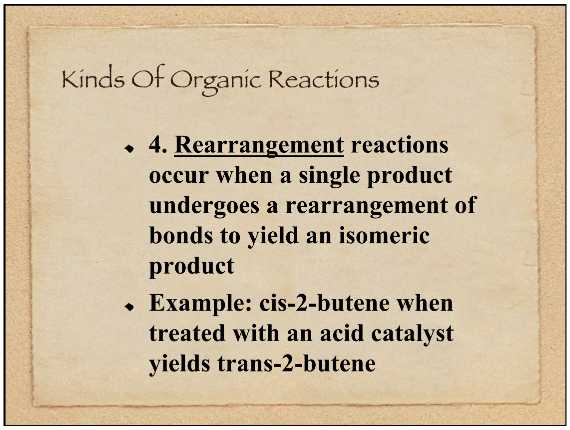
- 2. **Elimination** reactions occur when a single reactant splits into two products.

$CH_3 - CH_2Cl \rightarrow CH_2 = CH_2 + HCl$

Kinds Of Organic Reactions

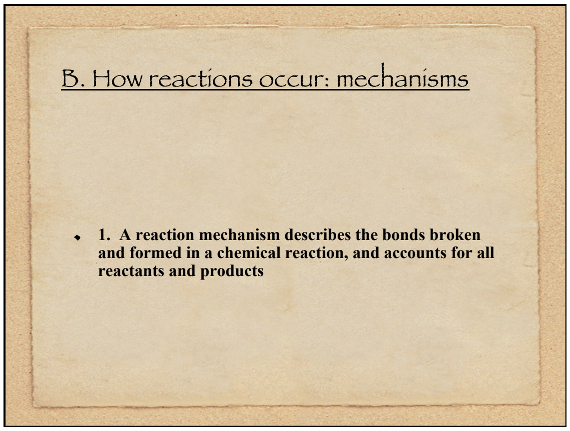
- 3. **Substitution** reactions occur when two reactants exchange parts to yield two new products.

$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$



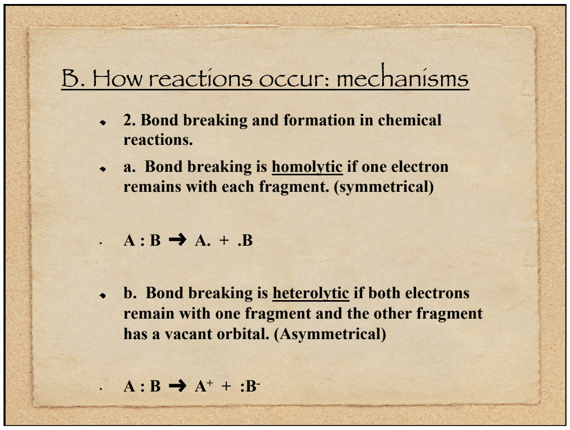
Kinds Of Organic Reactions

- 4. **Rearrangement reactions occur when a single product undergoes a rearrangement of bonds to yield an isomeric product**
- **Example: cis-2-butene when treated with an acid catalyst yields trans-2-butene**



B. How reactions occur: mechanisms

- **1. A reaction mechanism describes the bonds broken and formed in a chemical reaction, and accounts for all reactants and products**



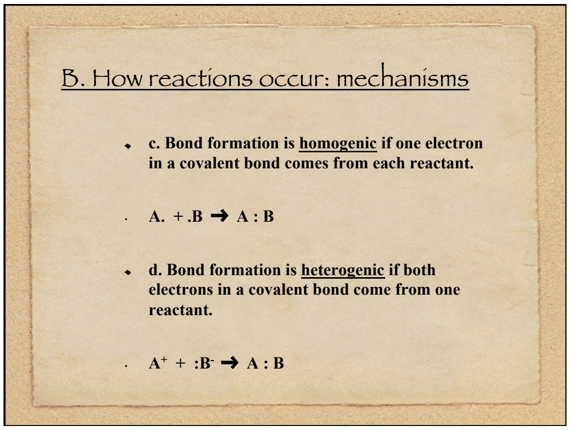
B. How reactions occur: mechanisms

- **2. Bond breaking and formation in chemical reactions.**
- **a. Bond breaking is homolytic if one electron remains with each fragment. (symmetrical)**

$A : B \rightarrow A. + .B$

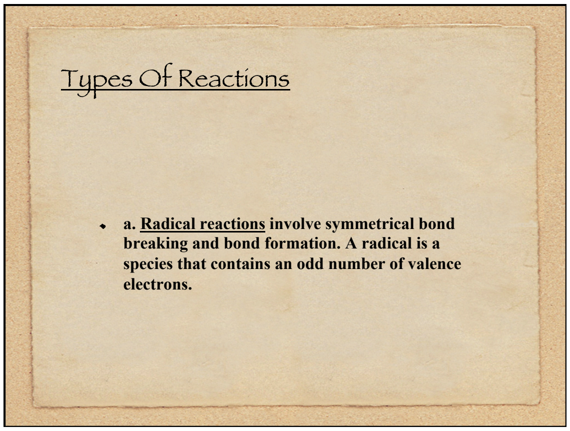
- **b. Bond breaking is heterolytic if both electrons remain with one fragment and the other fragment has a vacant orbital. (Asymmetrical)**

$A : B \rightarrow A^+ + :B^-$



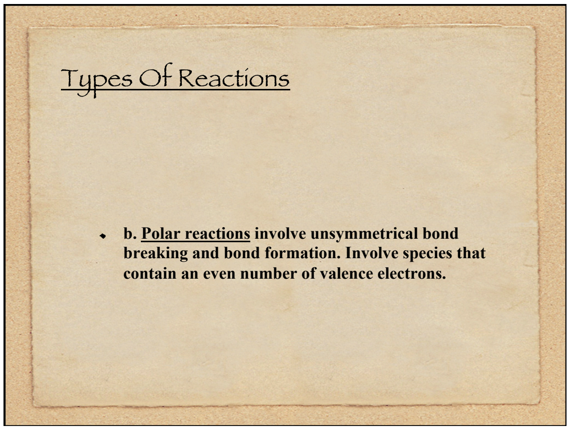
B. How reactions occur: mechanisms

- c. Bond formation is <u>homogenic</u> if one electron in a covalent bond comes from each reactant.
- A. + .B ➜ A : B
- d. Bond formation is <u>heterogenic</u> if both electrons in a covalent bond come from one reactant.
- A^+ + $:B^-$ ➜ A : B



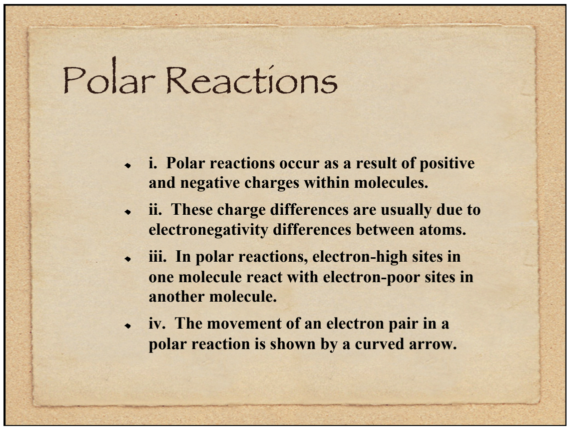
Types Of Reactions

- a. <u>Radical reactions</u> involve symmetrical bond breaking and bond formation. A radical is a species that contains an odd number of valence electrons.



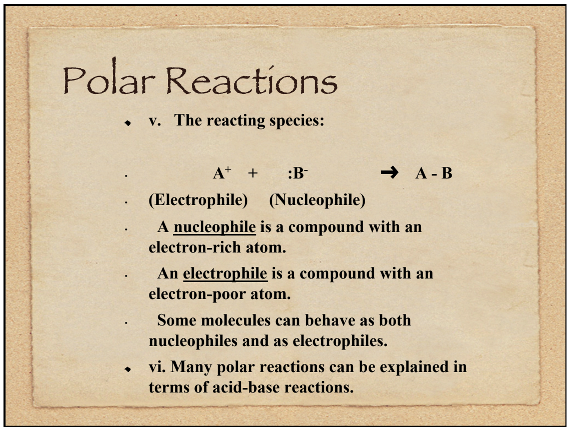
Types Of Reactions

- b. <u>Polar reactions</u> involve unsymmetrical bond breaking and bond formation. Involve species that contain an even number of valence electrons.



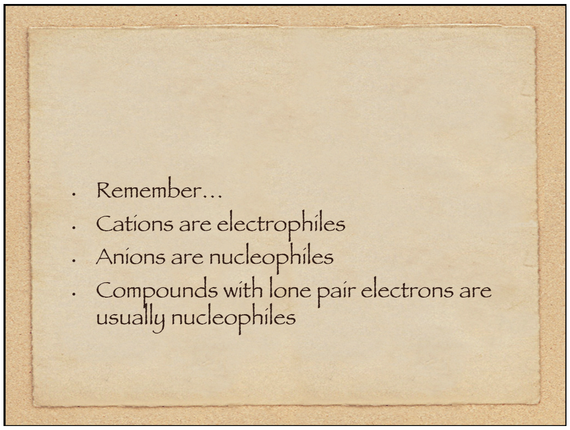
Polar Reactions

- **i. Polar reactions occur as a result of positive and negative charges within molecules.**
- **ii. These charge differences are usually due to electronegativity differences between atoms.**
- **iii. In polar reactions, electron-high sites in one molecule react with electron-poor sites in another molecule.**
- **iv. The movement of an electron pair in a polar reaction is shown by a curved arrow.**



Polar Reactions

- **v. The reacting species:**
  - $A^+ \quad + \quad :B^- \quad \rightarrow \quad A - B$
  - **(Electrophile) (Nucleophile)**
  - **A <u>nucleophile</u> is a compound with an electron-rich atom.**
  - **An <u>electrophile</u> is a compound with an electron-poor atom.**
  - **Some molecules can behave as both nucleophiles and as electrophiles.**
- **vi. Many polar reactions can be explained in terms of acid-base reactions.**



- Remember…
- Cations are electrophiles
- Anions are nucleophiles
- Compounds with lone pair electrons are usually nucleophiles

Try These ....

- Read sections 3.5, 3.6 (pages84-89)
- Do 3.10, 3.13
- Do 3.11, 3.12

Addition of HCl to ethylene

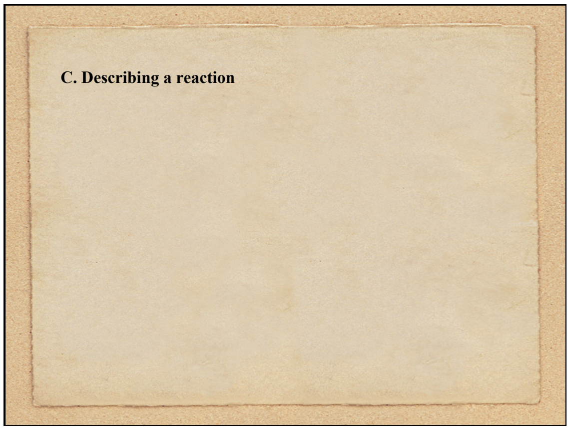
$CH_2 = CH_2 + HCl \rightarrow CH_3 - CH_2Cl$

- **a. This reaction is known as an electrophilic addition.**
- **b. The electrons in ethylene behave as a nucleophile.**
- **c. The reaction begins by the addition of the electrophile H^+ to the double bond.**
- **d. The resulting intermediate carbocation reacts with Cl^- to form chloroethane.**

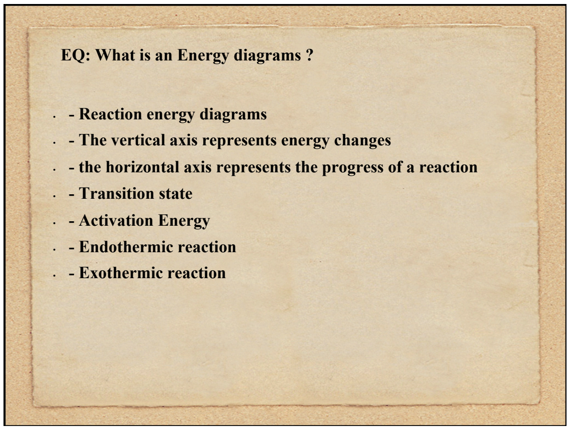
- **Refer to Fig 3.6 on page 91**

Show the reaction mechanism for the following reaction

$CH_2 = CH_2 + HCl \rightarrow CH_3 - CH_2Cl$

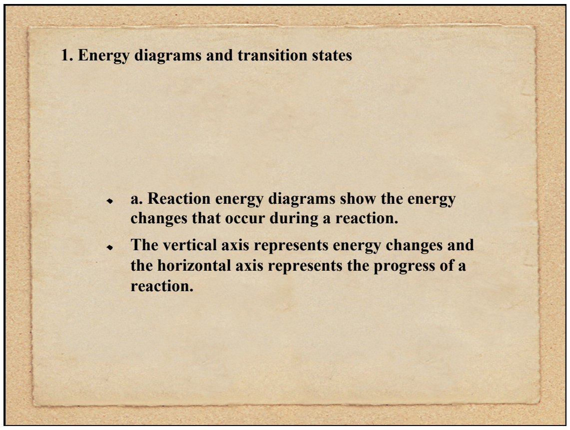


C. Describing a reaction



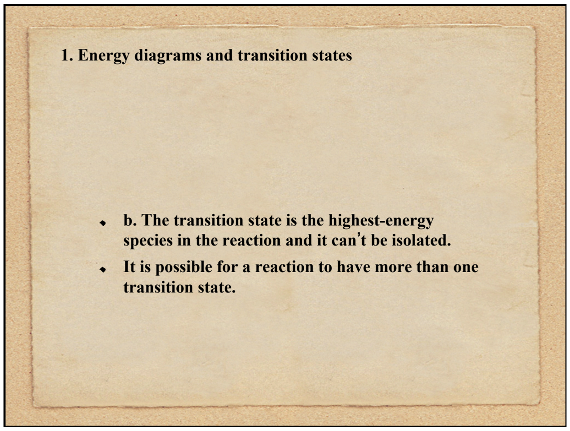
EQ: What is an Energy diagrams ?

- - Reaction energy diagrams
- - The vertical axis represents energy changes
- - the horizontal axis represents the progress of a reaction
- - Transition state
- - Activation Energy
- - Endothermic reaction
- - Exothermic reaction



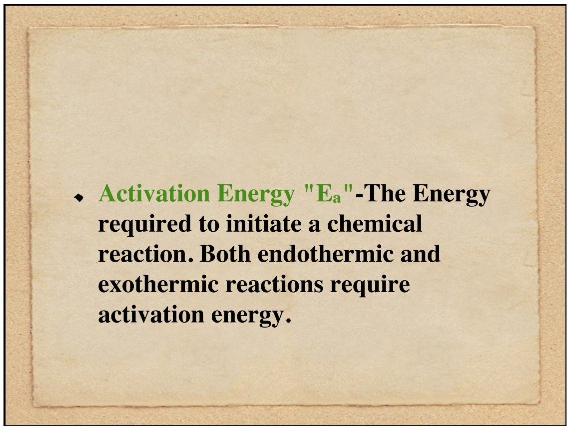
1. Energy diagrams and transition states

- a. Reaction energy diagrams show the energy changes that occur during a reaction.
- The vertical axis represents energy changes and the horizontal axis represents the progress of a reaction.

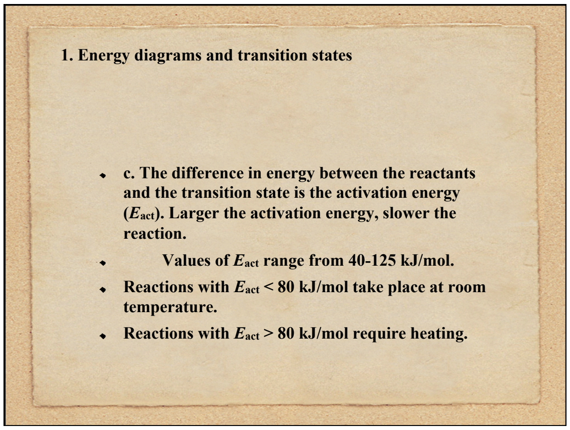


1. Energy diagrams and transition states

- b. The transition state is the highest-energy species in the reaction and it can't be isolated.
- It is possible for a reaction to have more than one transition state.

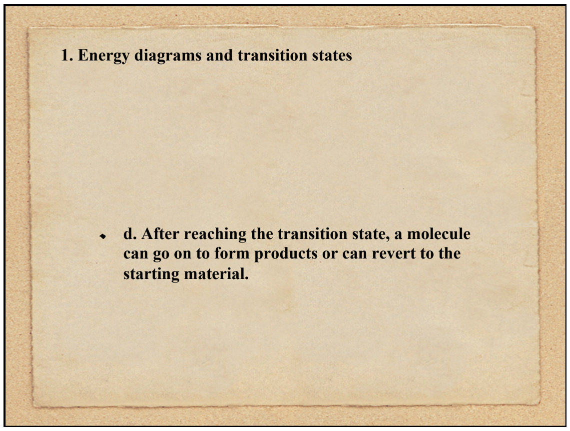


- Activation Energy "E_a"-The Energy required to initiate a chemical reaction. Both endothermic and exothermic reactions require activation energy.



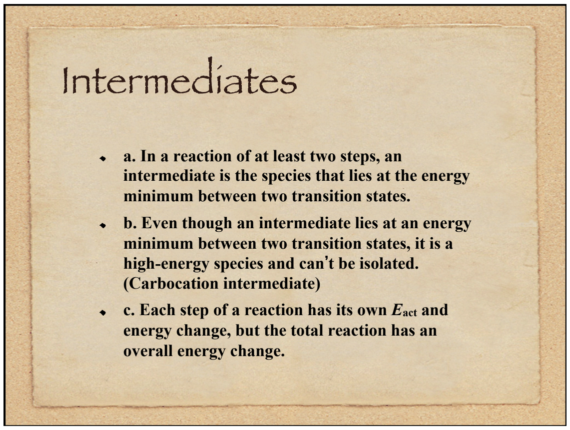
1. Energy diagrams and transition states

- **c. The difference in energy between the reactants and the transition state is the activation energy (E_{act}). Larger the activation energy, slower the reaction.**
- **Values of E_{act} range from 40-125 kJ/mol.**
- **Reactions with E_{act} < 80 kJ/mol take place at room temperature.**
- **Reactions with E_{act} > 80 kJ/mol require heating.**



1. Energy diagrams and transition states

- **d. After reaching the transition state, a molecule can go on to form products or can revert to the starting material.**



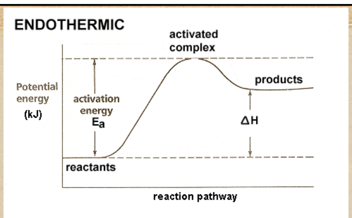
Intermediates

- **a. In a reaction of at least two steps, an intermediate is the species that lies at the energy minimum between two transition states.**
- **b. Even though an intermediate lies at an energy minimum between two transition states, it is a high-energy species and can't be isolated. (Carbocation intermediate)**
- **c. Each step of a reaction has its own E_{act} and energy change, but the total reaction has an overall energy change.**

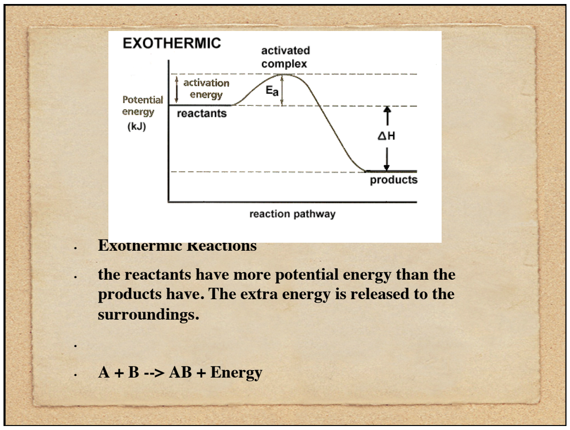
Energy change that takes place during a reaction can be described by considering

- **RATE (how fast the reaction occurs)**
- **Equilibria (how much the reaction occurs) The equilibrium position of a reaction is determined by H, the energy change.**
- **Endothermic reaction: energy is absorbed and the reaction has an unfavorable equilibrium constant.**
- **Exothermic reaction: energy is given off and the reaction has an favorable equilibrium constant.**

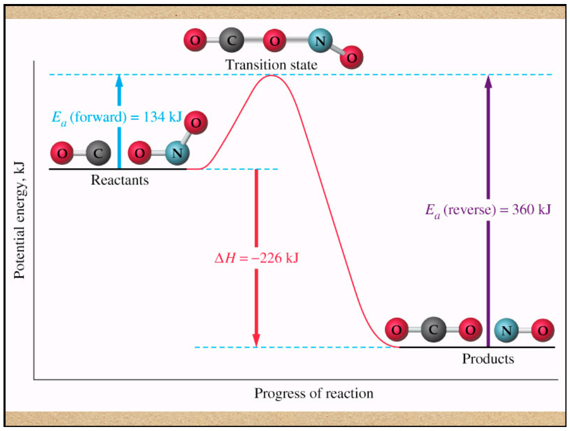
- **Try these …..**
- 3.16-3.18, 3.52, 3.53, 3.54, 3.55, 3.56, 3.57, 3.58, 3.59, 3.60

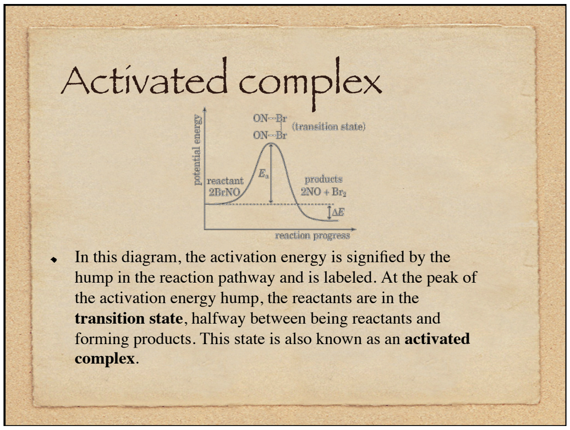


- **Endothermic Reactions**
- **the reactants have less potential energy than do the products. Energy must be input in order to raise the particles up to the higher energy level.**
- **Energy + A + B --> AB**



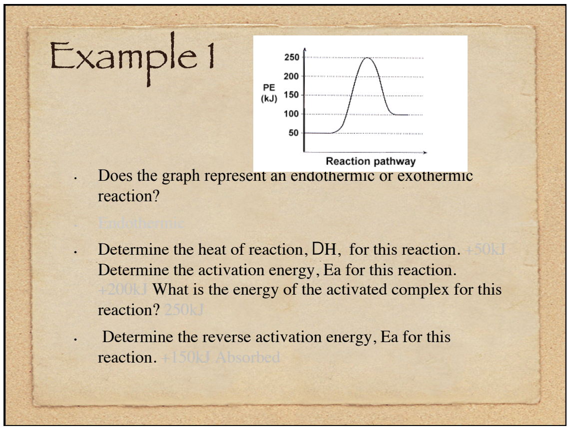
- Exothermic Reactions
- the reactants have more potential energy than the products have. The extra energy is released to the surroundings.
- A + B --> AB + Energy





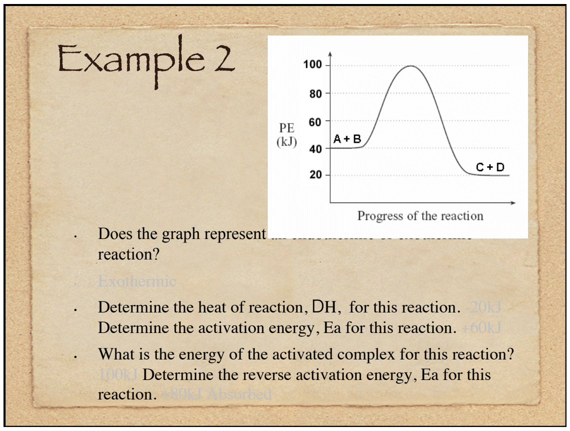
Activated complex

- In this diagram, the activation energy is signified by the hump in the reaction pathway and is labeled. At the peak of the activation energy hump, the reactants are in the **transition state**, halfway between being reactants and forming products. This state is also known as an **activated complex**.



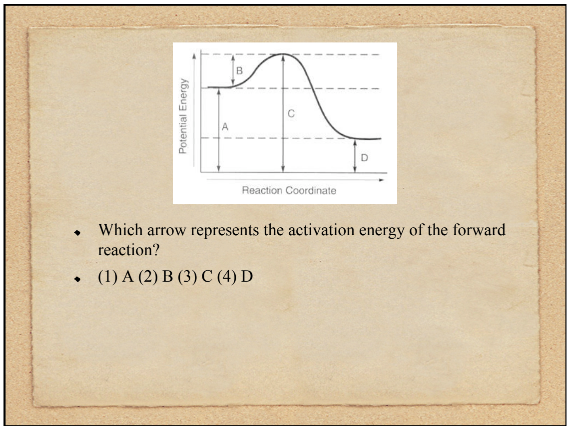
Example 1

- Does the graph represent an endothermic or exothermic reaction?
- Endothermic
- Determine the heat of reaction, DH, for this reaction. +50kJ Determine the activation energy, Ea for this reaction. +200kJ What is the energy of the activated complex for this reaction? 250kJ
- Determine the reverse activation energy, Ea for this reaction. +150kJ Absorbed



Example 2

- Does the graph represent
reaction?
- Exothermic
- Determine the heat of reaction, DH, for this reaction. -20kJ Determine the activation energy, Ea for this reaction. +60kJ
- What is the energy of the activated complex for this reaction? 100kJ Determine the reverse activation energy, Ea for this reaction. +80kJ Absorbed



- Which arrow represents the activation energy of the forward reaction?
- (1) A (2) B (3) C (4) D