Chapter 5

Alkenes Structure, Nomenclature, and an introduction to Reactivity • Thermodynamics and Kinetics

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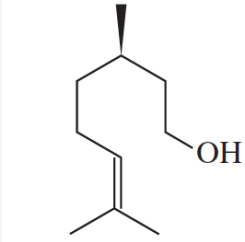
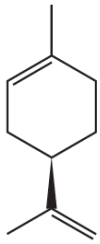
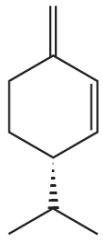
Alkenes



citronellol
in rose and geranium oils



limonene
in lemon and orange oils



β-phellandrene
oil of eucalyptus

Saturated and Unsaturated Hydrocarbons

$CH_3CH_2CH_2CH_3$
an alkane
a saturated hydrocarbon

$CH_3CH{=}CHCH_3$
an alkene
an unsaturated hydrocarbon

Saturated hydrocarbons have no double bonds.

Unsaturated hydrocarbons have one or more double bonds.

Nomenclature of Alkenes

	$H_2C{=}CH_2$	$CH_3CH{=}CH_2$		
systematic name:	ethene	propene	cyclopentene	cyclohexene
common name:	ethylene	propylene		

Replace "ane" of alkane with "ene."

$^{4}CH_3{}^{3}CH_2{}^{2}CH{=}{}^{1}CH_2$ — 1-butene

$^{1}CH_3{}^{2}CH{=}{}^{3}CH{}^{4}CH_3$ — 2-butene

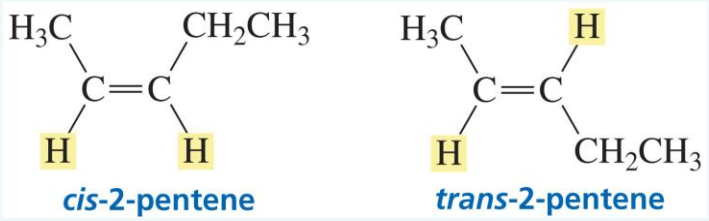
$^{1}CH_3{}^{2}CH{=}{}^{3}CH{}^{4}CH_2{}^{5}CH_2{}^{6}CH_3$ — 2-hexene

The functional group gets the lowest possible number.

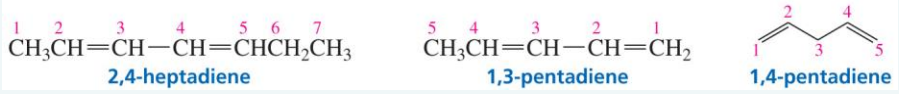
$^{6}CH_3{}^{5}CH_2{}^{4}CH_2{}^{3}CH_2{}^{2}C(=CH_2)CH_2CH_2CH_3$ (1 CH_2)

2-propyl-1-hexene

Stereoisomers of an Alkene are named using a *cis* or *trans* Prefix

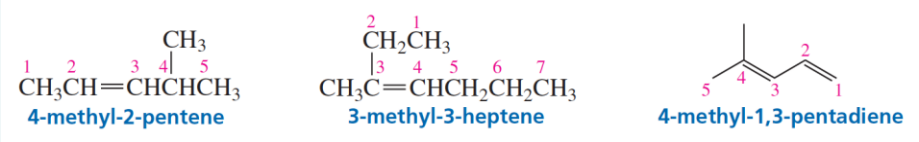


Nomenclature of Dienes



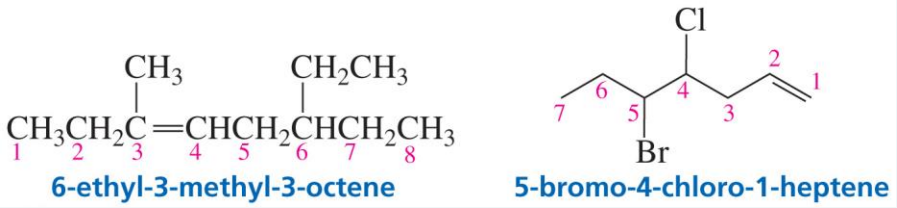
two double bonds = diene

Nomenclature of Alkenes



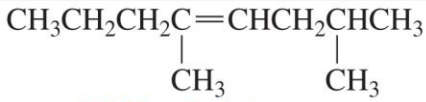
Number in the direction so that the functional group gets the lowest number.

Nomenclature of Alkenes

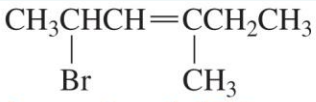


Substituents are stated in alphabetical order.

Nomenclature of Alkenes

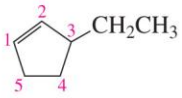


2,5-dimethyl-4-octene
not
4,7-dimethyl-4-octene
because 2 < 4

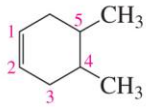


2-bromo-4-methyl-3-hexene
not
5-bromo-3-methyl-3-hexene
because 2 < 3

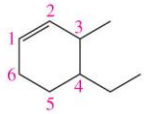
Nomenclature of Cyclic Alkenes



3-ethylcyclopentene



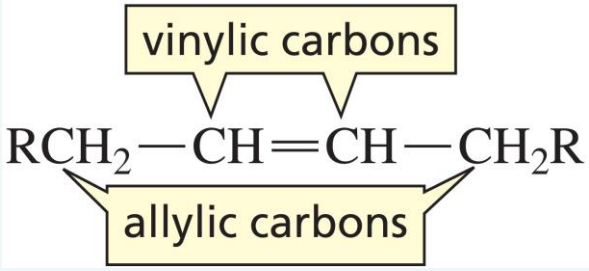
4,5-dimethylcyclohexene



4-ethyl-3-methylcyclohexene

A number is not needed to denote the position of the functional group; it is always between C1 and C2.

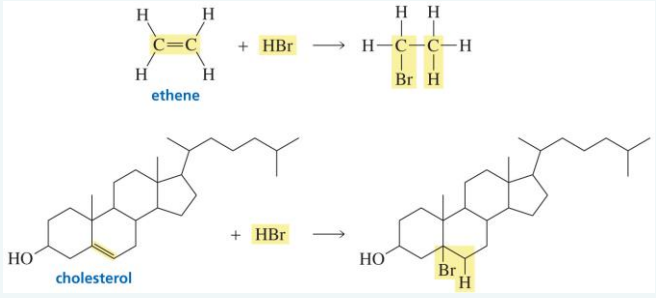
Vinylic and Allylic Carbons



vinylic carbon: the sp^2 carbon of an alkene

allylic carbon: a carbon adjacent to a vinylic carbon

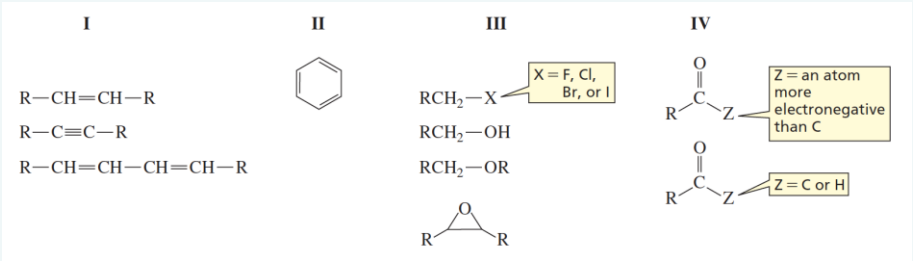
Reactions of Organic Compounds



Organic compounds can be divided into families.

All members of a family react in the same way. The family a compound belongs to depends on its functional group.

Each family can be put in one of four Groups



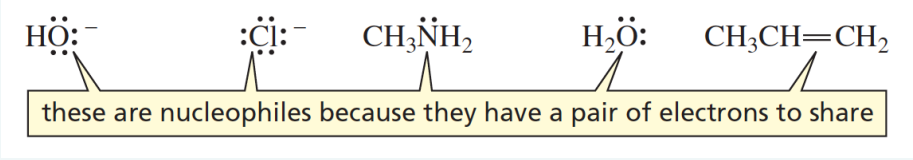
The families in a group react in similar ways.

Electrophiles

these are electrophiles because they have a positive charge

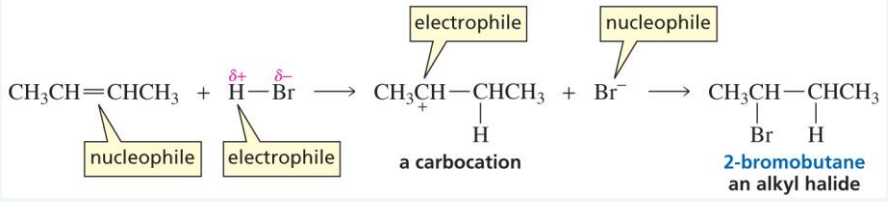
H^+ $CH_3\overset{+}{C}H_2$

Nucleophiles



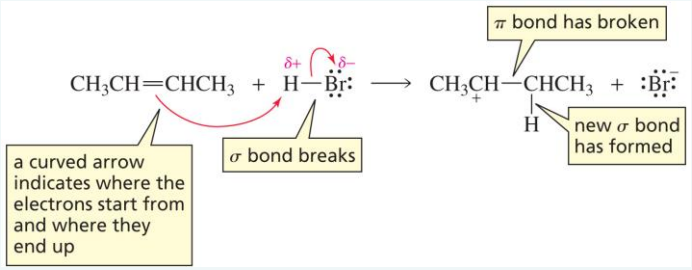
A nucleophile has
- a negative charge
- a lone pair
- a double bond

A Nucleophile reacts with an Electrophile



Your first organic reaction is a two-step reaction.

Curved Arrows

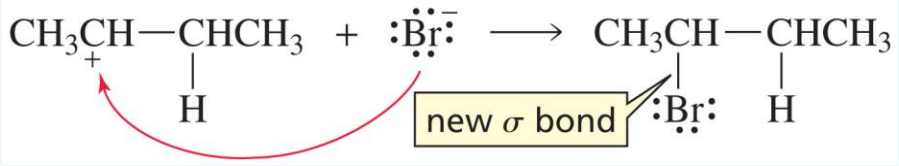


first step of the reaction

Curved arrows are used to show the mechanism of a reaction.

The mechanism of a reaction is the step-by-step description of the process by which reactants are converted into products.

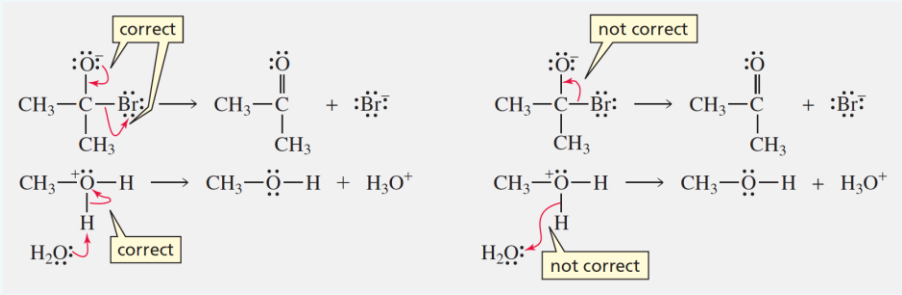
Curved Arrows



second step of the reaction

The curved arrow shows where the electrons start from and where they end up.

How to draw Curved Arrows



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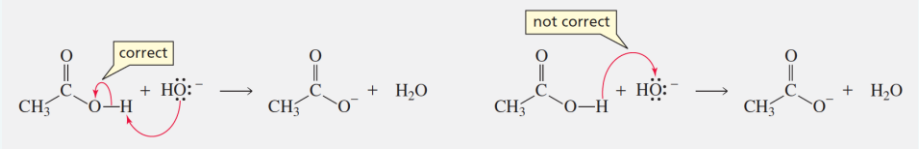

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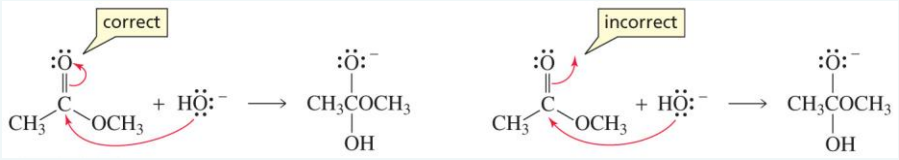

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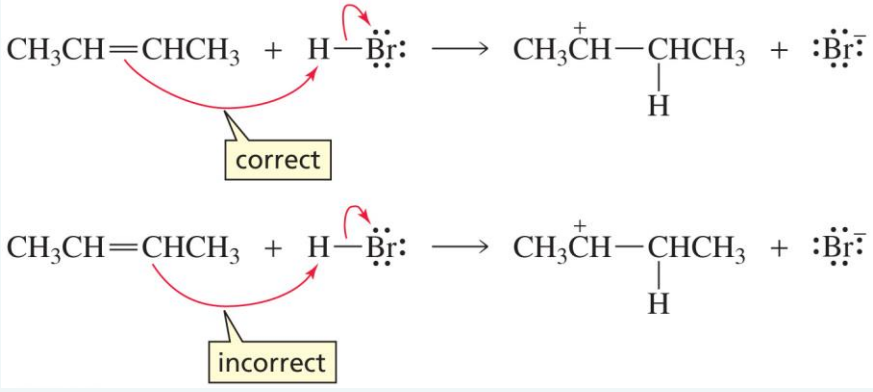
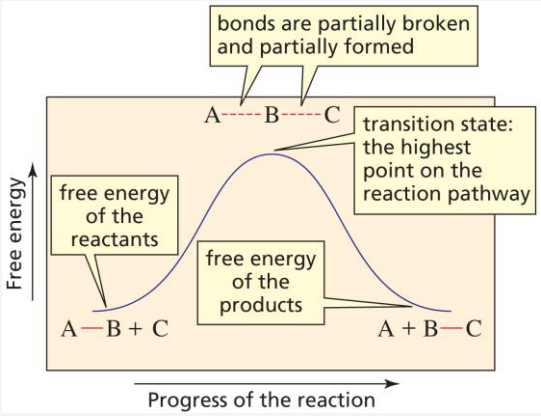
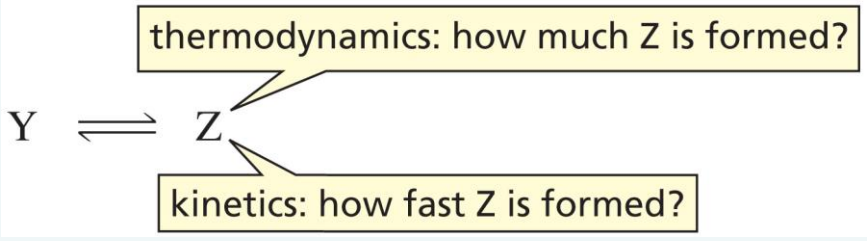


A Reaction Coordinate Diagram



A reaction coordinate diagram shows the energy changes that take place in each step of a reaction.

Thermodynamics and Kinetics



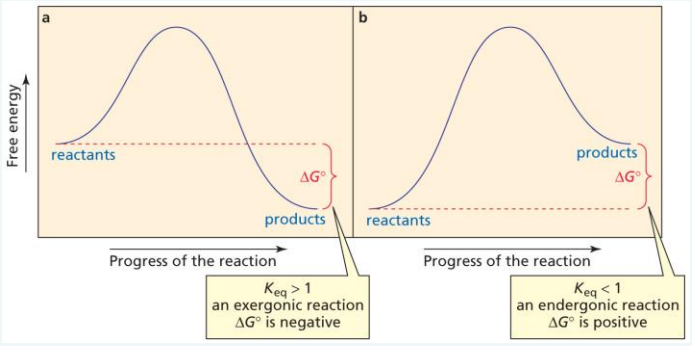
The Equilibrium Constant

$$A + B \rightleftharpoons C + D$$

$$K_{eq} = \frac{[\text{products}]}{[\text{reactants}]} = \frac{[C][D]}{[A][B]}$$

The equilibrium constant gives the concentration of reactants and products at equilibrium.

Exergonic and Endergonic Reactions



$$\Delta G^\circ = -RT \ln K_{eq}$$

Gibbs Free-Energy Change (ΔG°)

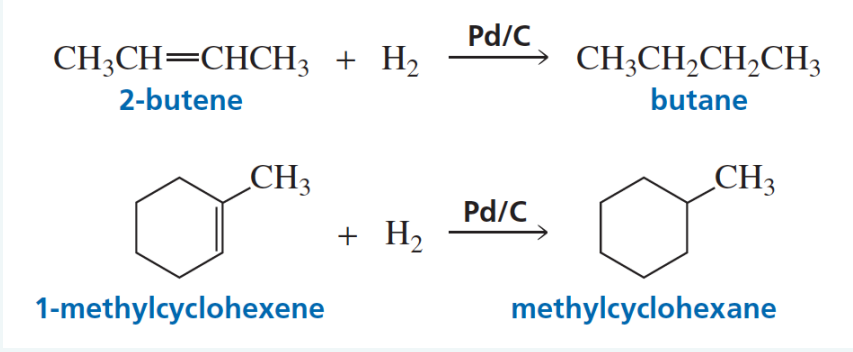
$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$$

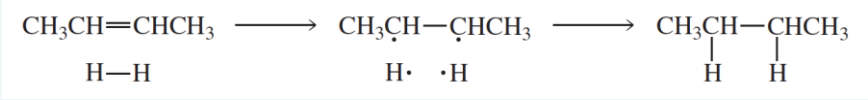
ΔG° = free energy of the products – free energy of the reactants

ΔH° = heat required to break bones – heat released from forming bonds

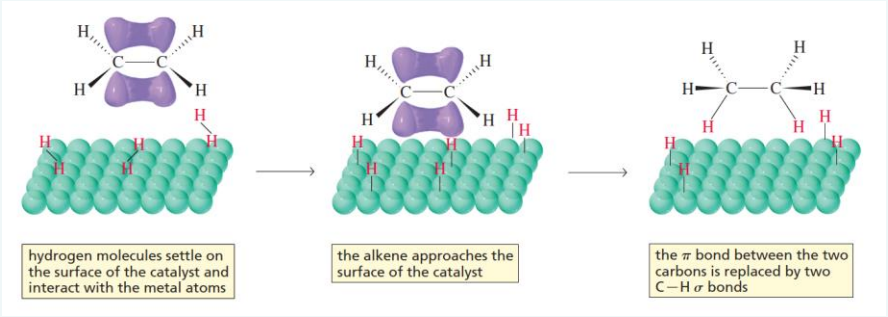
ΔS° = freedom of motion of the products – freedom of motion of the reactants

A Reduction Reaction

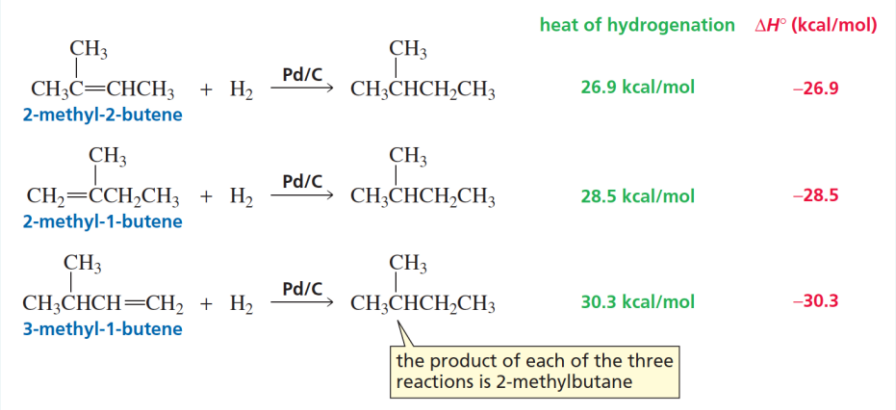




Catalytic Hydrogenation



Using $\Delta H°$ Values to determine the Relative Stabilities of Alkenes



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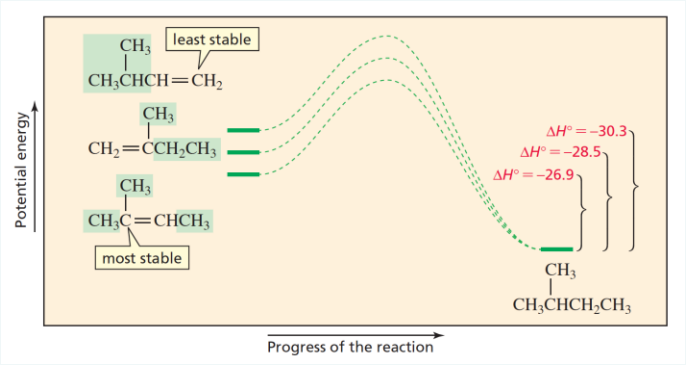
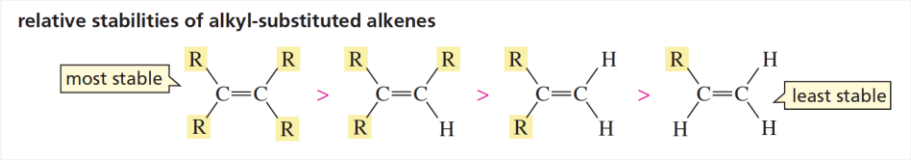
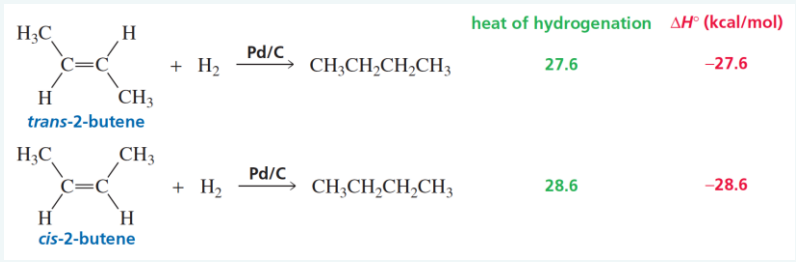


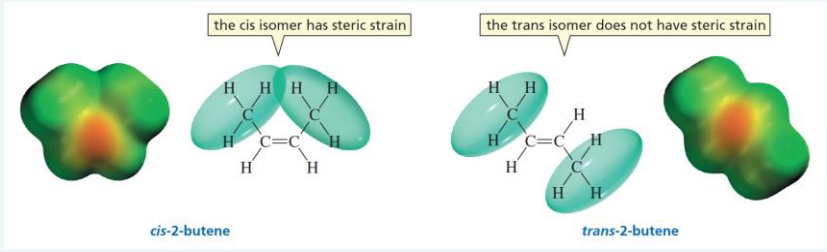
The relative energies (stabilities) of three alkenes that can be catalytically hydrogenated to 2-methylbutane. The most stable alkene has the smallest heat of hydrogenation. (Notice that when a reaction coordinate diagram shows ΔH° values, the *y*-axis is potential energy; when it shows ΔG° values, the *y*-axis is free energy [Figure 5.2].)

Relative Stabilities of Alkenes

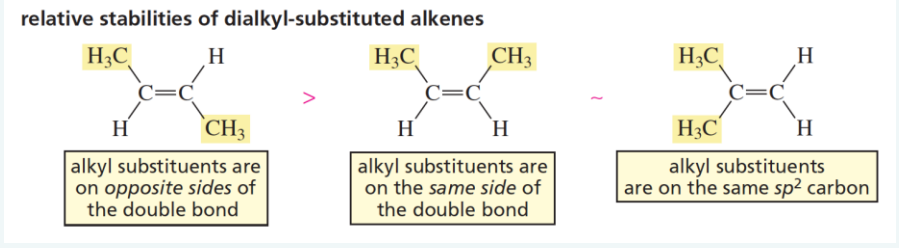


Relative Stabilities of Cis and Trans Alkenes

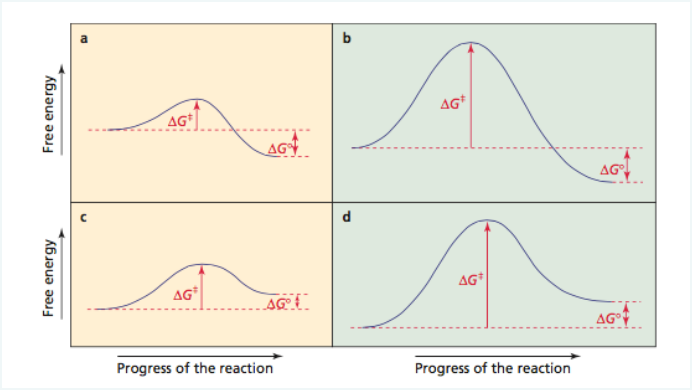




Relative Stabilities of Dialkyl-Substituted Alkenes



Kinetics: How fast is the product formed?



$\Delta G^{\ddagger}$ = free energy of the transition state - free energy of the reactants

The greater the energy barrier, the slower the reaction.

Rate of a Reaction

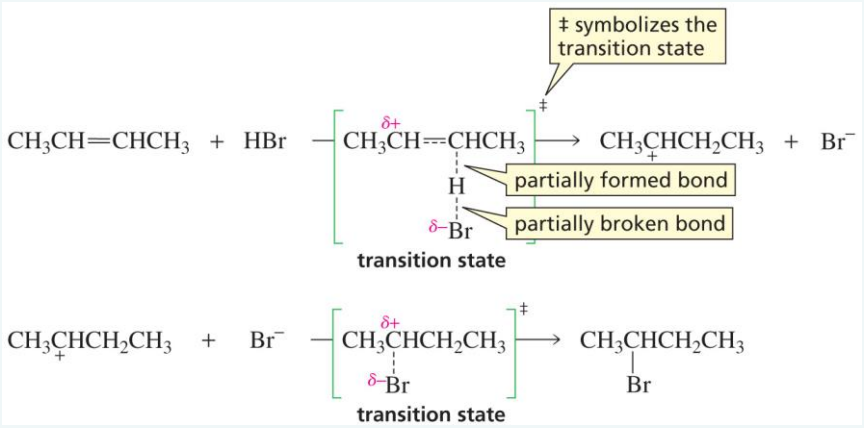
$$\text{rate of a reaction} = \left(\begin{array}{c}\text{number of collisions}\\ \text{per unit of time}\end{array}\right) \times \left(\begin{array}{c}\text{fraction with}\\ \text{sufficient energy}\end{array}\right) \times \left(\begin{array}{c}\text{fraction with}\\ \text{proper orientation}\end{array}\right)$$

Increasing the concentration increases the rate.

Increasing the temperature increases the rate.

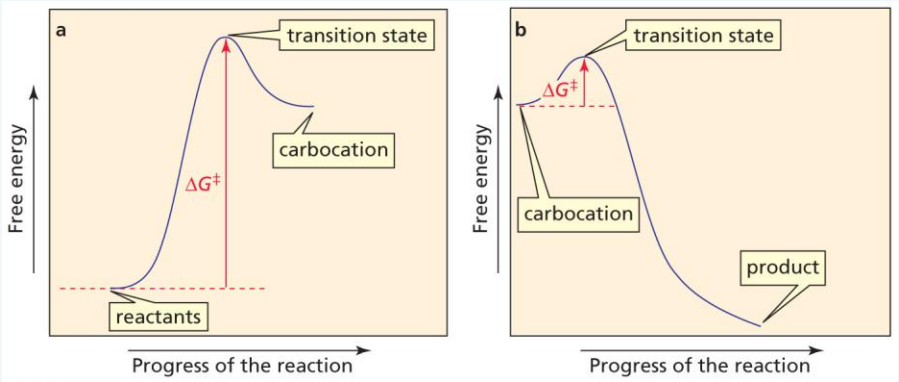
The rate can also be increased by a catalyst.

An Electrophilic Addition Reaction

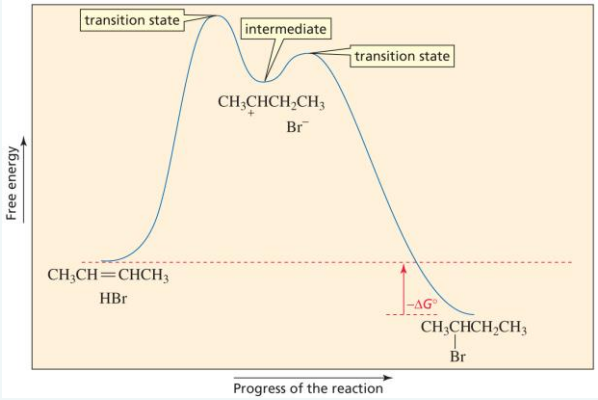


Transition states have partially formed bonds.

Reaction Coordinate Diagram for each step of the addition of HBr to 2-Butene



Reaction Coordinate Diagram for the addition of HBr to 2-Butene



The rate-limiting step of the reaction is the step that has its transition state at the highest point of the reaction coordinate diagram.

A Catalyst

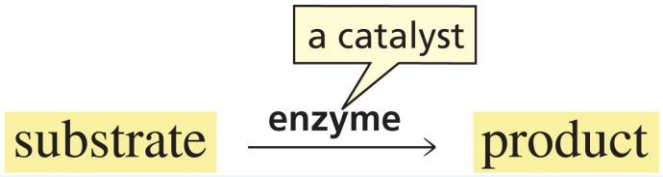
A catalyst provides a pathway for a reaction with a lower energy barrier.

A catalyst does not change the energy of the starting point (the reactants) or the energy of the end point (the products).

Enzymes

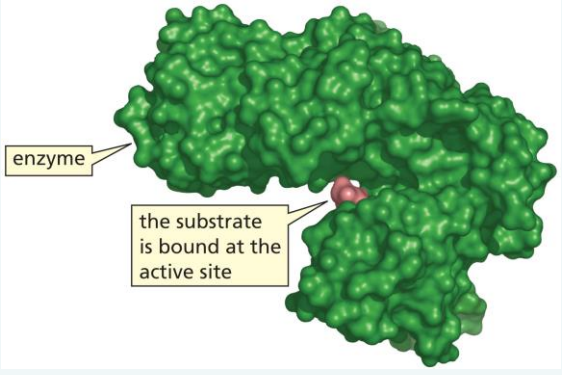
Most biological reactions require a catalyst.

Most biological catalysts are proteins called enzymes.



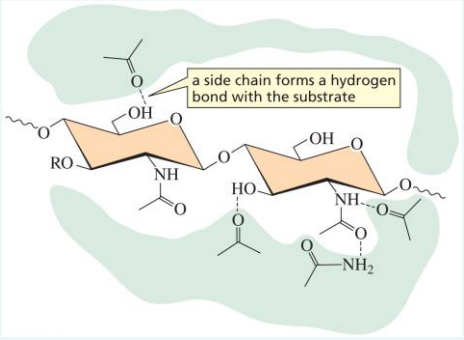
The reactant of a biological reaction is called a substrate.

The Active Site of an Enzyme



An enzyme binds its substrate at its active site.

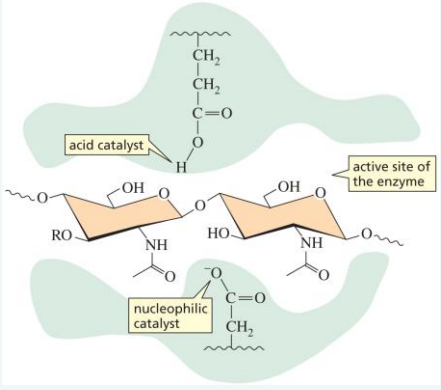
Enzyme Side Chains that bind the Substrate



Some enzyme side chains bind the substrate.

Some enzyme side chains are acids, bases, and nucleophiles that catalyze the reaction.

Enzyme Side Chains that catalyze the Reaction



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