



# **Reaction Mechanism**

*Prof. Dr. Chiara Valsecchi*

# Class Goals

- Understand what is the mechanism of a chemical reaction
- Understand what can affect the speed of a reaction

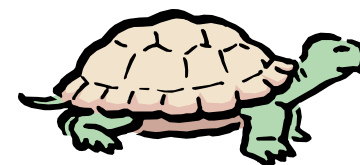
# Reaction Mechanisms

The **sequence of events** that describes the actual process by which reactants become products.

Most reactions occur in a series of steps: the balanced equation does not tell us how the reaction occurs!

Each of these processes is known as an **elementary reaction** or step.

**Rate-determining step:** the slowest step in the mechanism



# Elementary Steps

- **Molecularity:** number of molecules present in an elementary step.

Unimolecular reaction      $A \longrightarrow \text{products}$       $\text{rate} = k [A]$

Bimolecular reaction      $A + B \longrightarrow \text{products}$       $\text{rate} = k [A][B]$

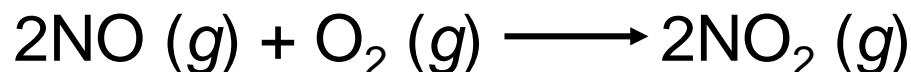
Bimolecular reaction      $A + A \longrightarrow \text{products}$       $\text{rate} = k [A]^2$

The order of a reaction can be written from the stoichiometric coefficients of the rate-determining step !!

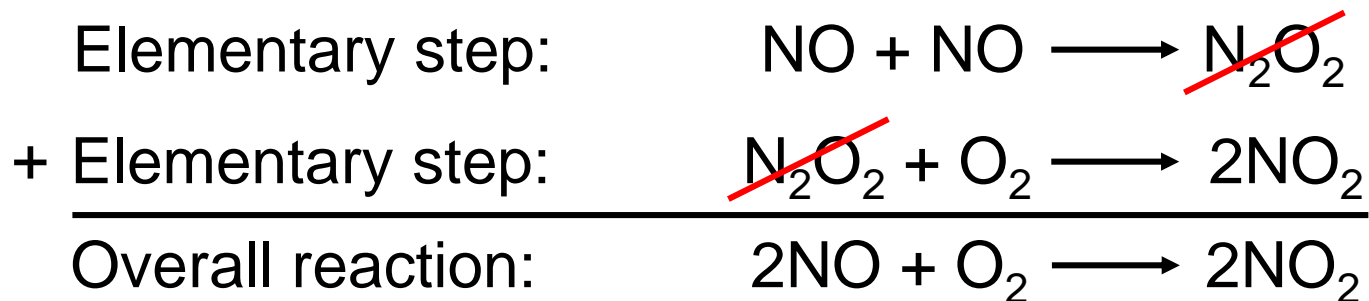
This is why stoichiometric coefficient of the total reaction sometimes do not match the reaction orders!

# Reaction Mechanism

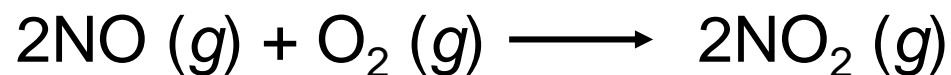
- The sum of the elementary steps **must** give the overall balanced equation for the reaction.
- The rate-determining step should predict the same rate law that is determined experimentally.



$\text{N}_2\text{O}_2$  is detected during the reaction!



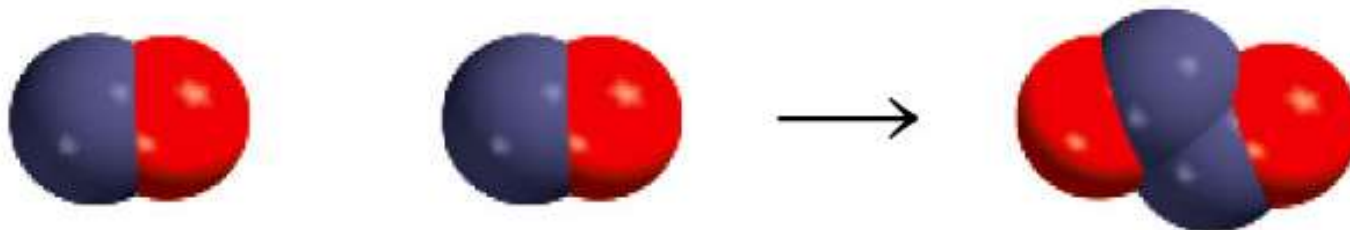
# Reaction Mechanism



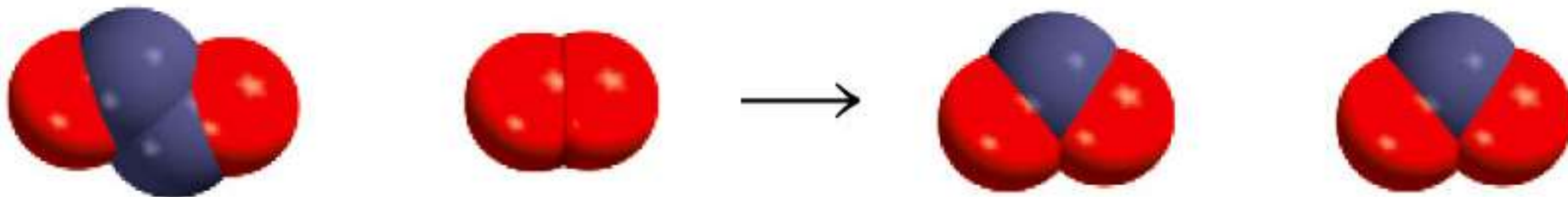
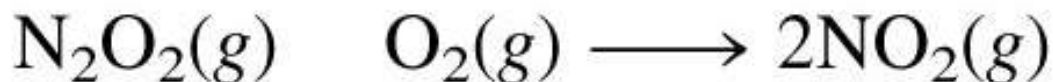
Step 1.



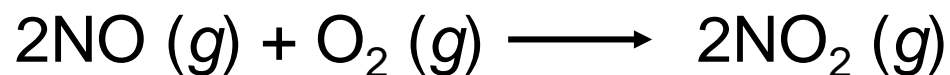
Rate-determining  
step



Step 2.



# Reaction Mechanism

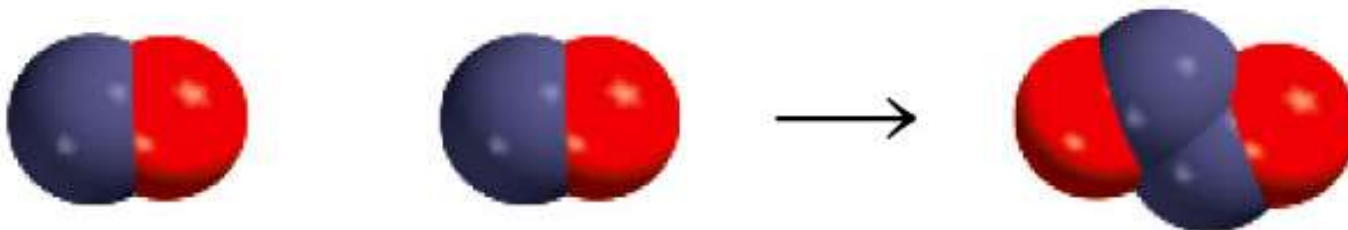


$$\text{rate} = k[\text{NO}_2]^2$$

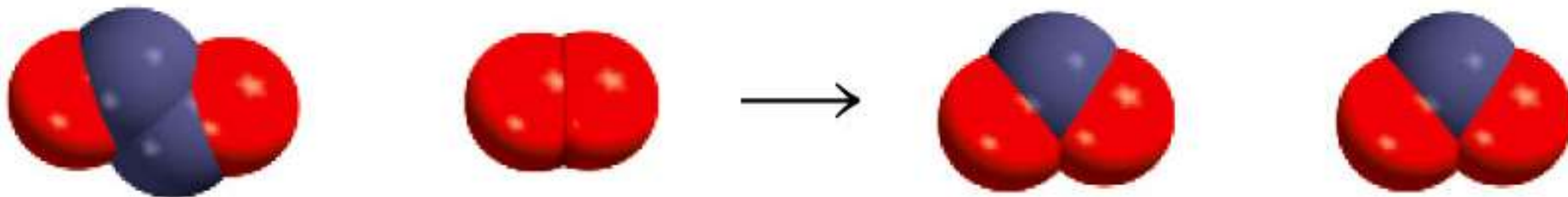
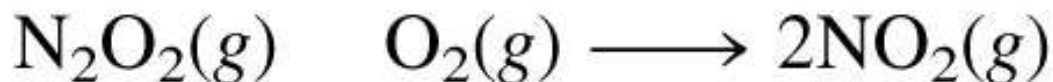
Step 1.



Rate-determining  
step



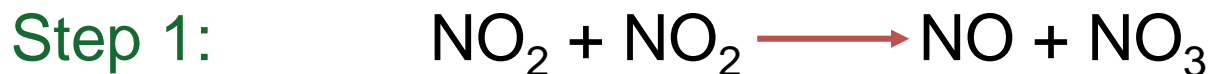
Step 2.



# Reaction Mechanism



The reaction is believed to occur via two steps:



What is the intermediate?



What can you say about step 1 ?

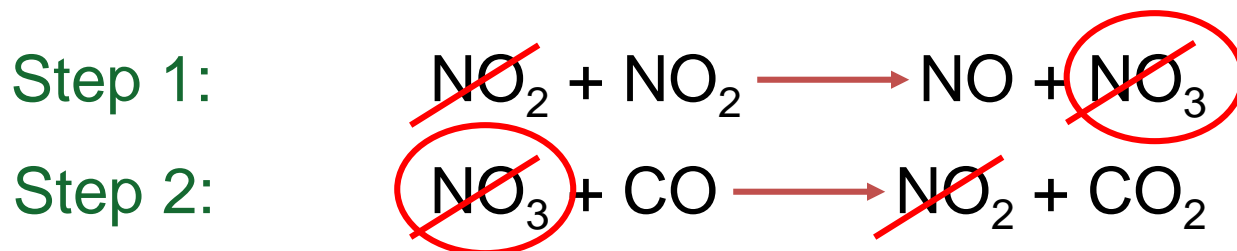
If the rate =  $k[\text{NO}_2]^2$  it means that step 1 is the slowest one



# Reaction Mechanism



The reaction is believed to occur via two steps:



What is the intermediate?



What can you say about step 1 ?

The rate =  $k[\text{NO}_2]^2$ . It means that step 1 is the slowest one

# What affect the Reaction Rate Constant

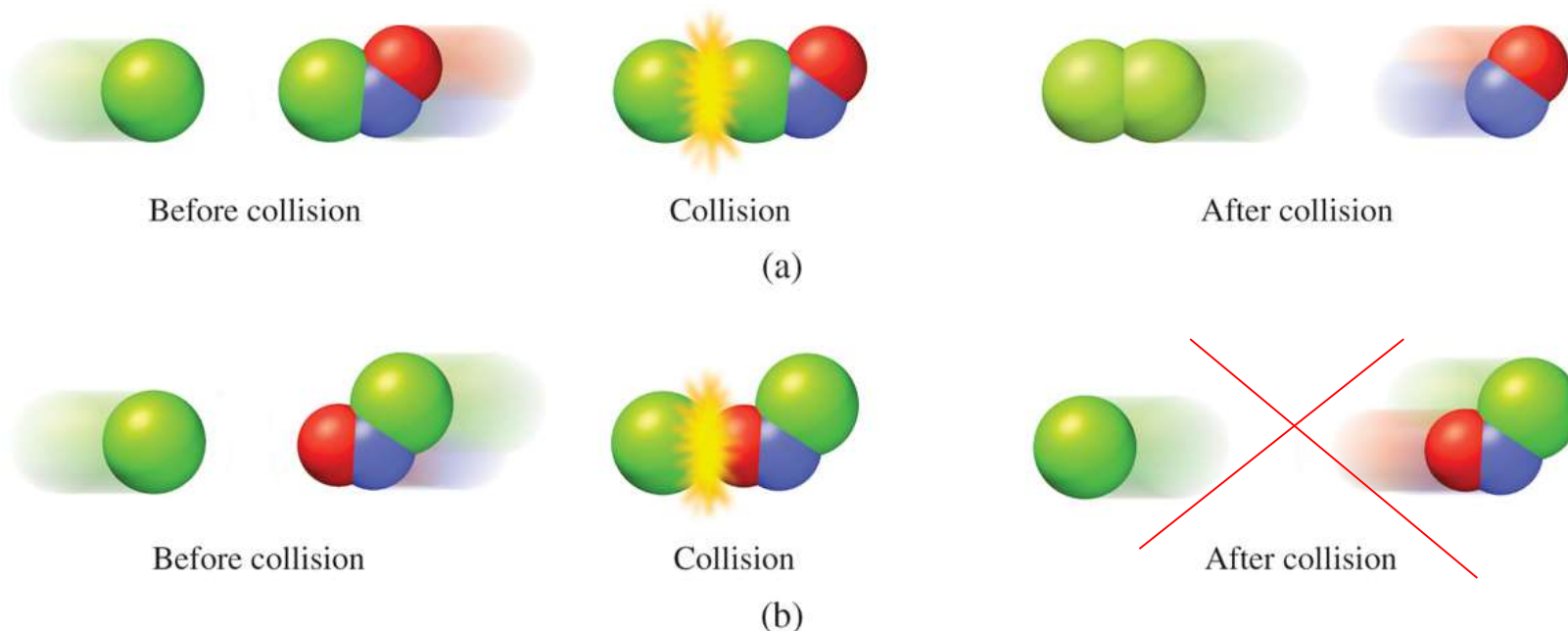
1. **Temperature:** At higher temperatures, reactant molecules have more kinetic energy, move faster, and collide more often and with greater energy
2. **Surface Area:** The amount of particles that are exposed.  
The greater the surface area the faster the reaction.
3. **Concentrations of reactants**  
As the concentration of reactants increases, so does the likelihood that reactant molecules will collide.
4. **Catalysts**  
Speed up reactions by lowering *activation energy*  
More area for reactants to be in contact

# What affect the Reaction Rate Constant

We need to understand two concepts from:

- **Collision Theory:** When two chemicals react, their molecules have to collide with each other (in a particular orientation) with sufficient energy for the reaction to take place.
- **Kinetic Theory:** Increasing temperature means the molecules move faster.

# Collision Theory



The molecules involved in the reaction have to interact with the right orientation, so more collision means more possibility to have the right approximation

# Collision Theory

Particles must collide in order to react

More frequency of collisions → higher the reaction rate

Only two particles may react at one time

Many factors must be met:

- Orientation

- Energy needed to break bonds (activation energy)



**Effective collisions:** a collision that does result in a reaction

An activated complex (transition state) forms in an effective collision

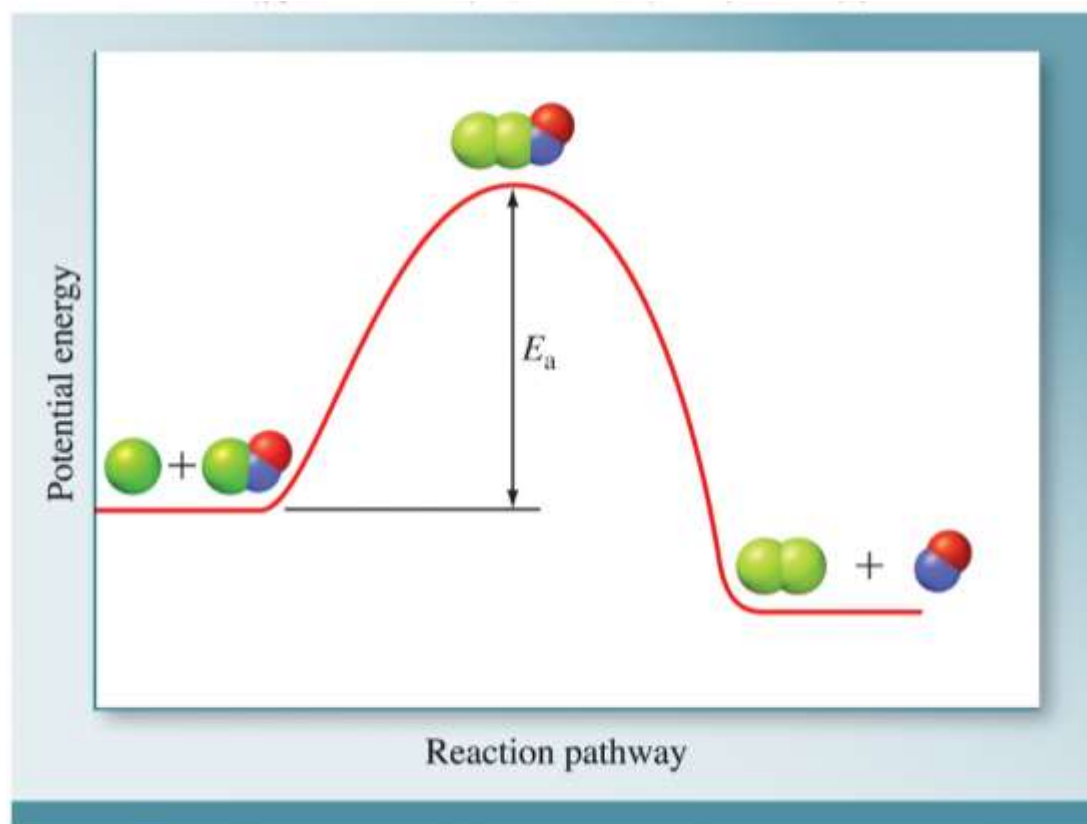
# Activation Energy

There is a minimum amount of energy required for a reaction: the **activation energy**,  $E_a$ .

A reaction cannot occur unless the molecules possess sufficient energy to get over the activation energy barrier.

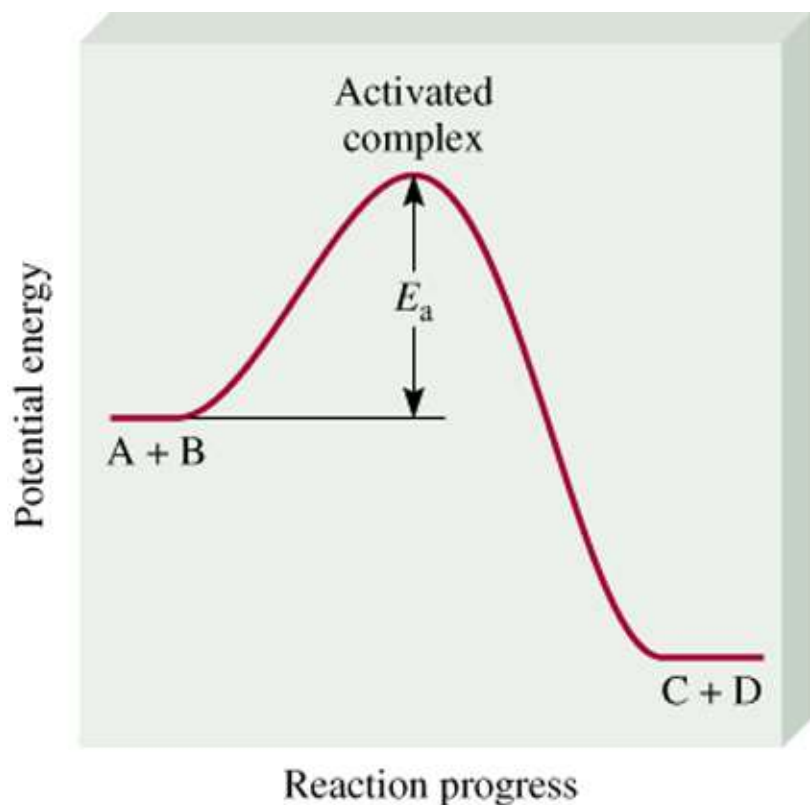


BREAK BONDS!

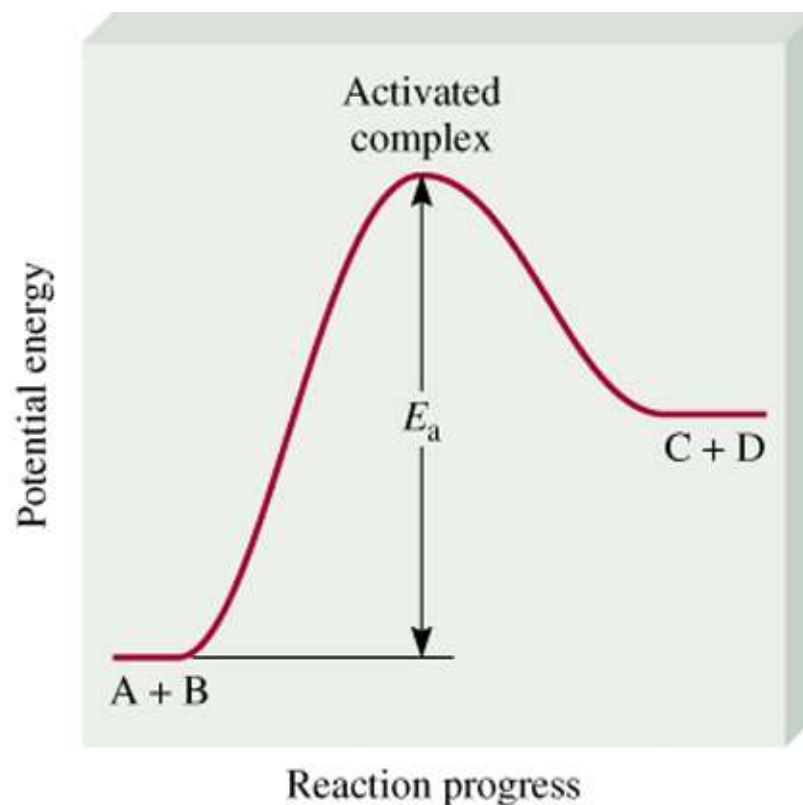


# Activation Energy

## Exothermic Reaction



## Endothermic Reaction




$E_a$  is the energy difference between the reagents and the intermediate state, **do not confuse**

# Arrhenius Equation

There is a mathematical relationship between  $k$  (*reaction rate constant*) and activation energy  $E_a$ :

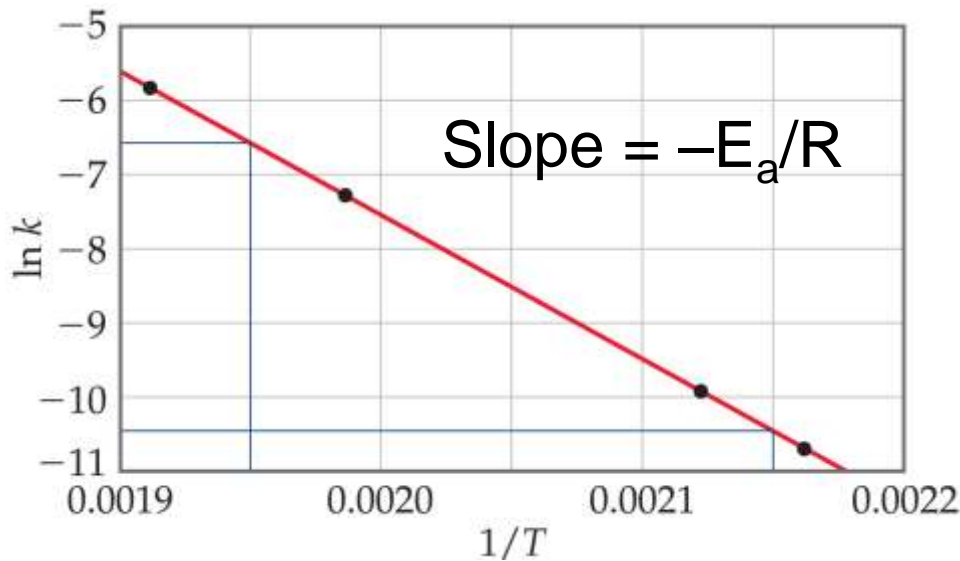
Rate =  $k [A][B]$


$$k = Ae^{-\frac{E_a}{RT}}$$

where  $A$  is the *frequency factor*, a number that represents the likelihood that collisions would occur with the proper orientation for reaction.



# Arrhenius Equation



Taking the natural logarithm of both sides, the equation becomes

$$\ln(k) = -\frac{E_a}{RT} + \ln A$$

$$y = mx + b$$

When  $k$  is determined experimentally at several temperatures,  $E_a$  can be calculated from the slope of a plot of  $\ln(k)$  vs.  $1/T$ .

# Catalysts and Reaction Rates

A **catalyst** is a substance that increases the rate of a chemical reaction without itself being consumed.

How do catalysts increase reaction rates?

In general, catalysts lower the  $E_a$  for a reaction:

- Catalysts can increase the number of effective collisions.
- Catalyst can provide a different mechanism for the reaction.

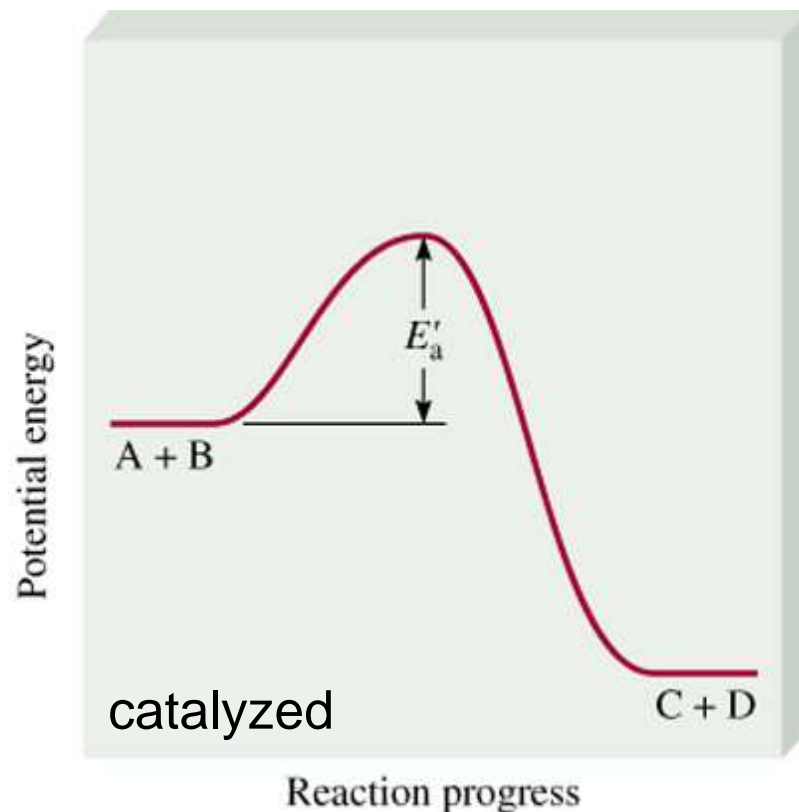
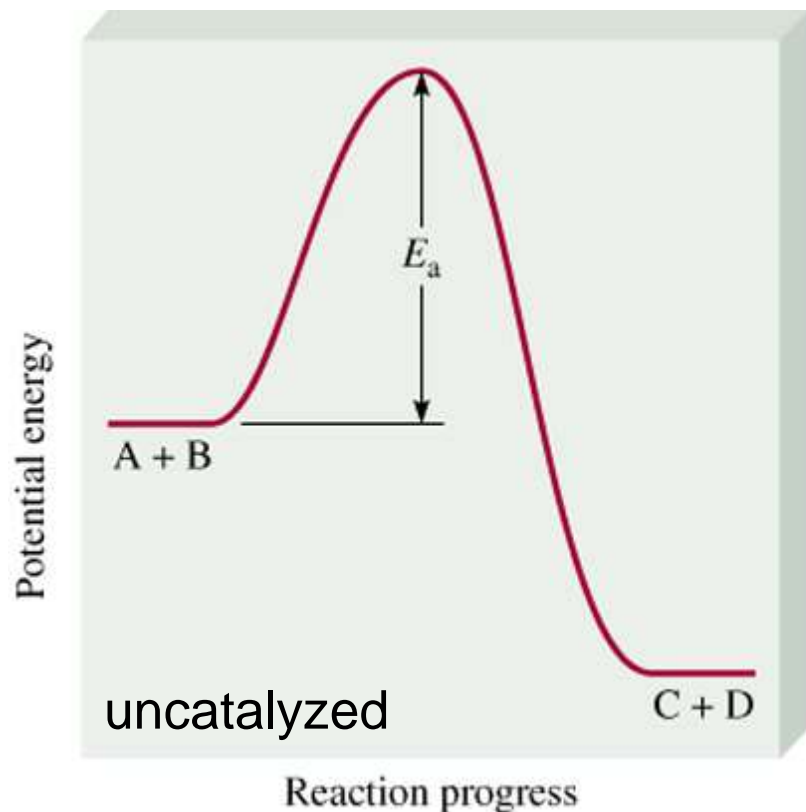
1. Keeps molecule close
2. Create favorable orientation for the reaction to happens

# Catalysts and Reaction Rates

$$E_a \downarrow$$

$$k \uparrow$$

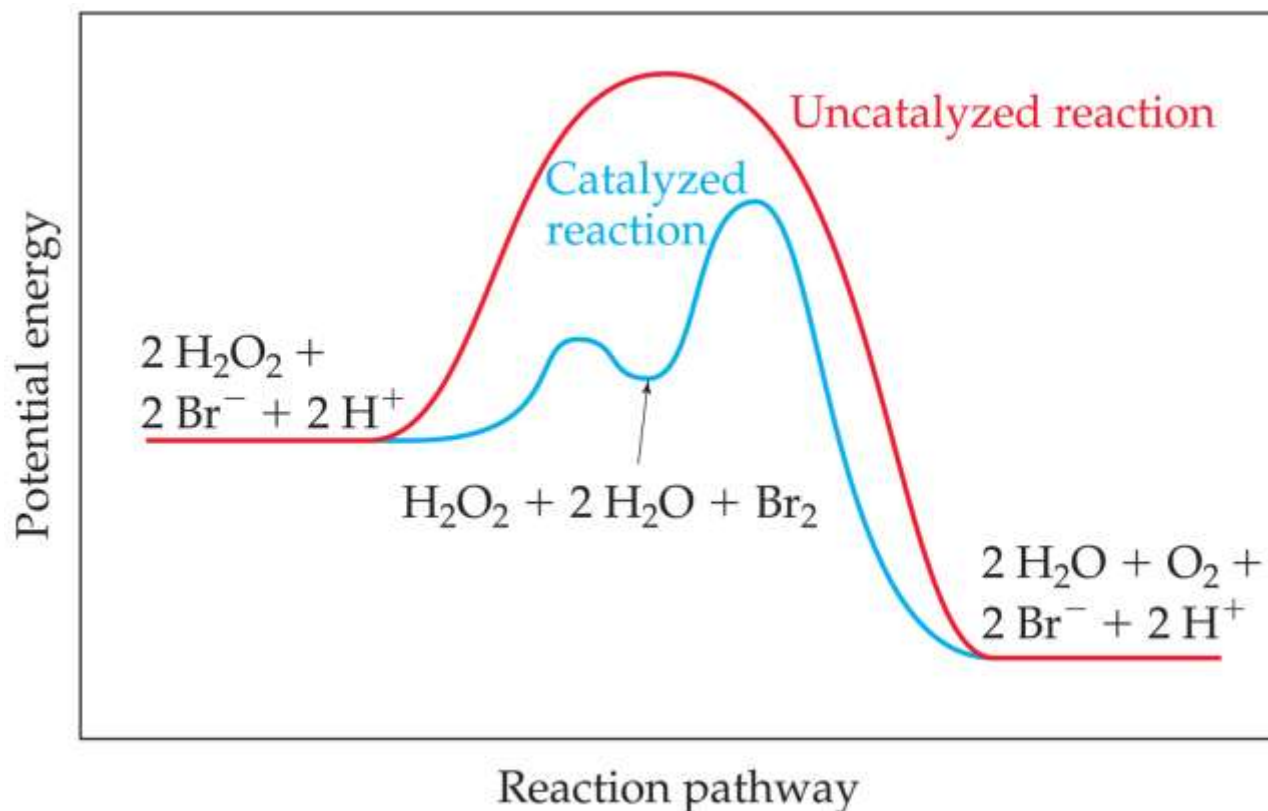
Lower  $E_a$



$$\text{rate}_{\text{catalyzed}} > \text{rate}_{\text{uncatalyzed}}$$

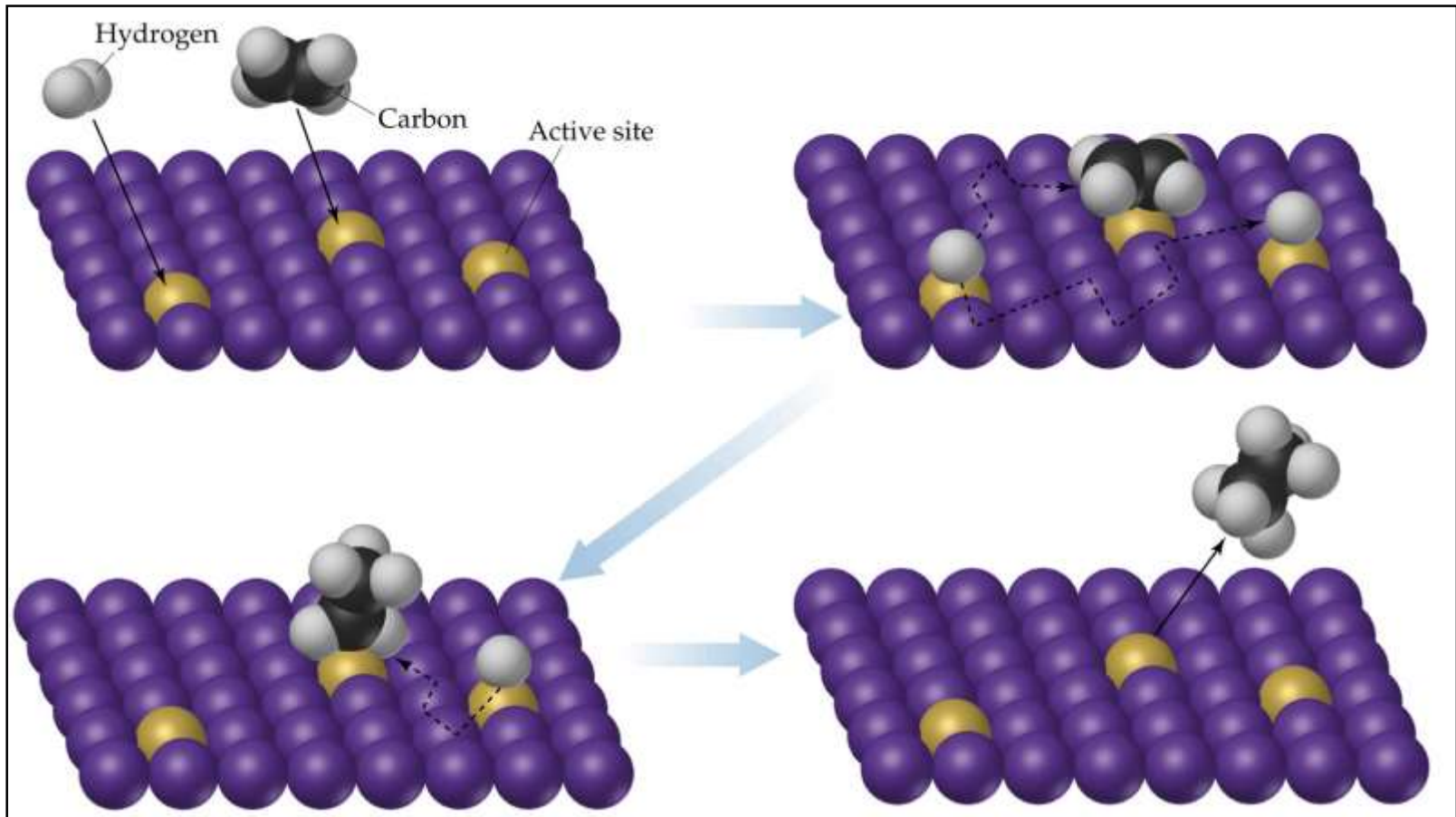
# Catalysts and Reaction Rates

Catalysts **change the mechanism** by which the process occurs.

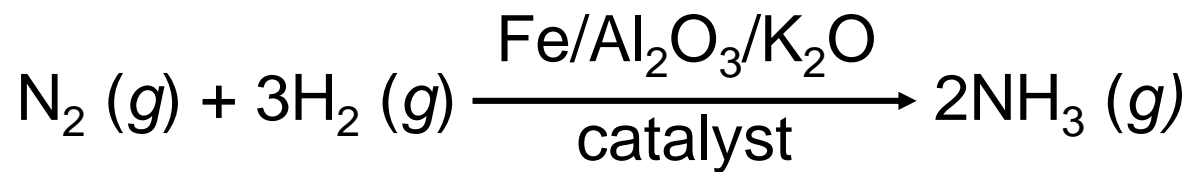
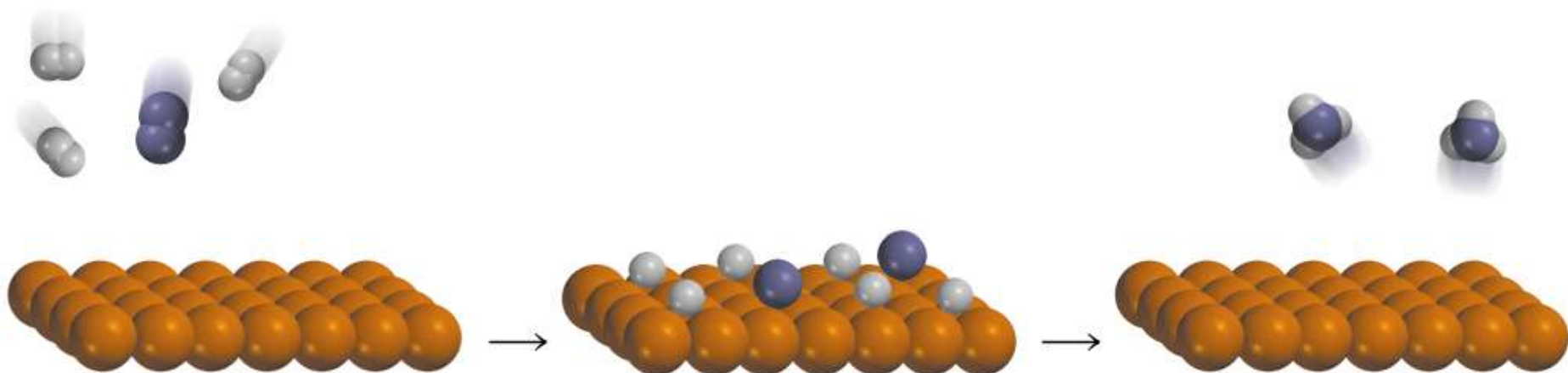


# Catalysts and Reaction Rates

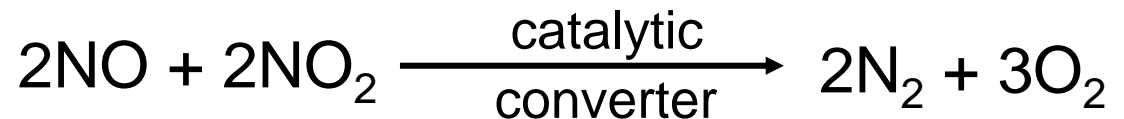
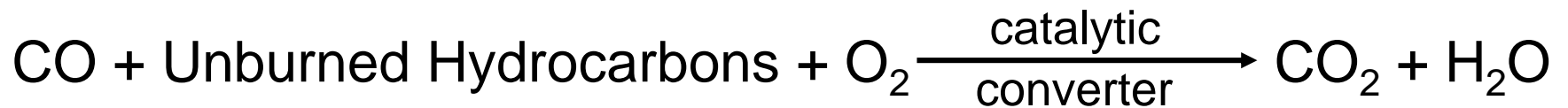
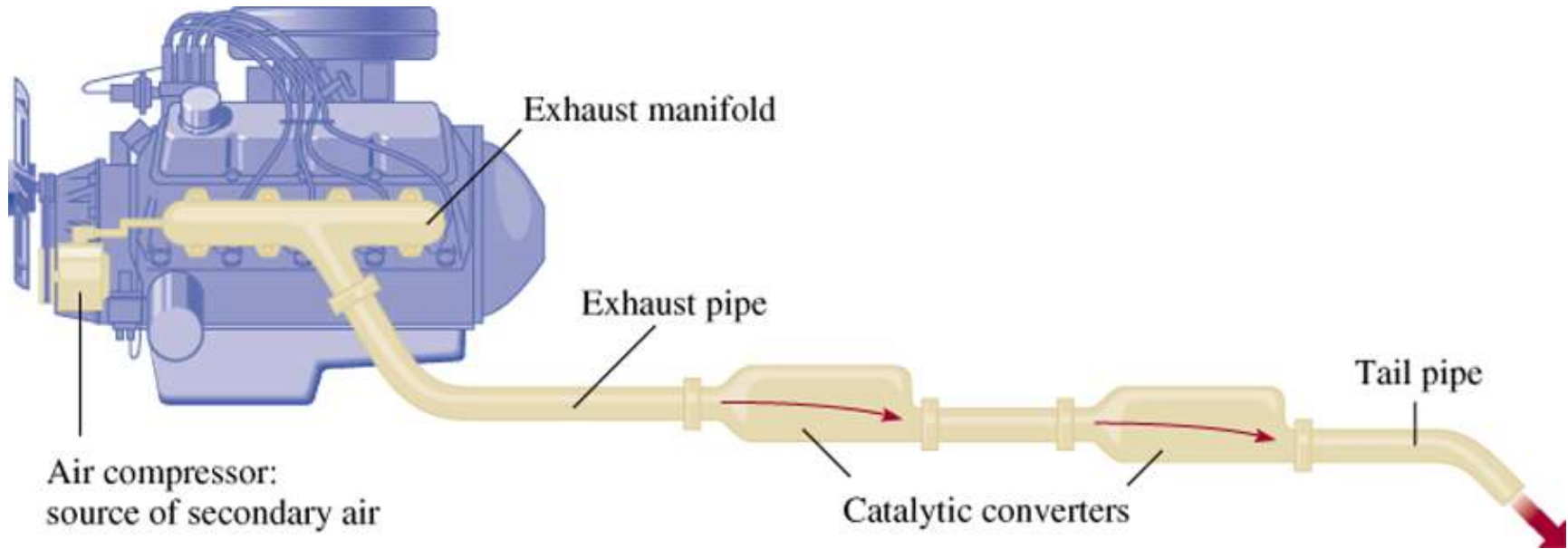
One way a catalyst can speed up a reaction is by holding the reactants together and helping bonds to break.



# Haber Process

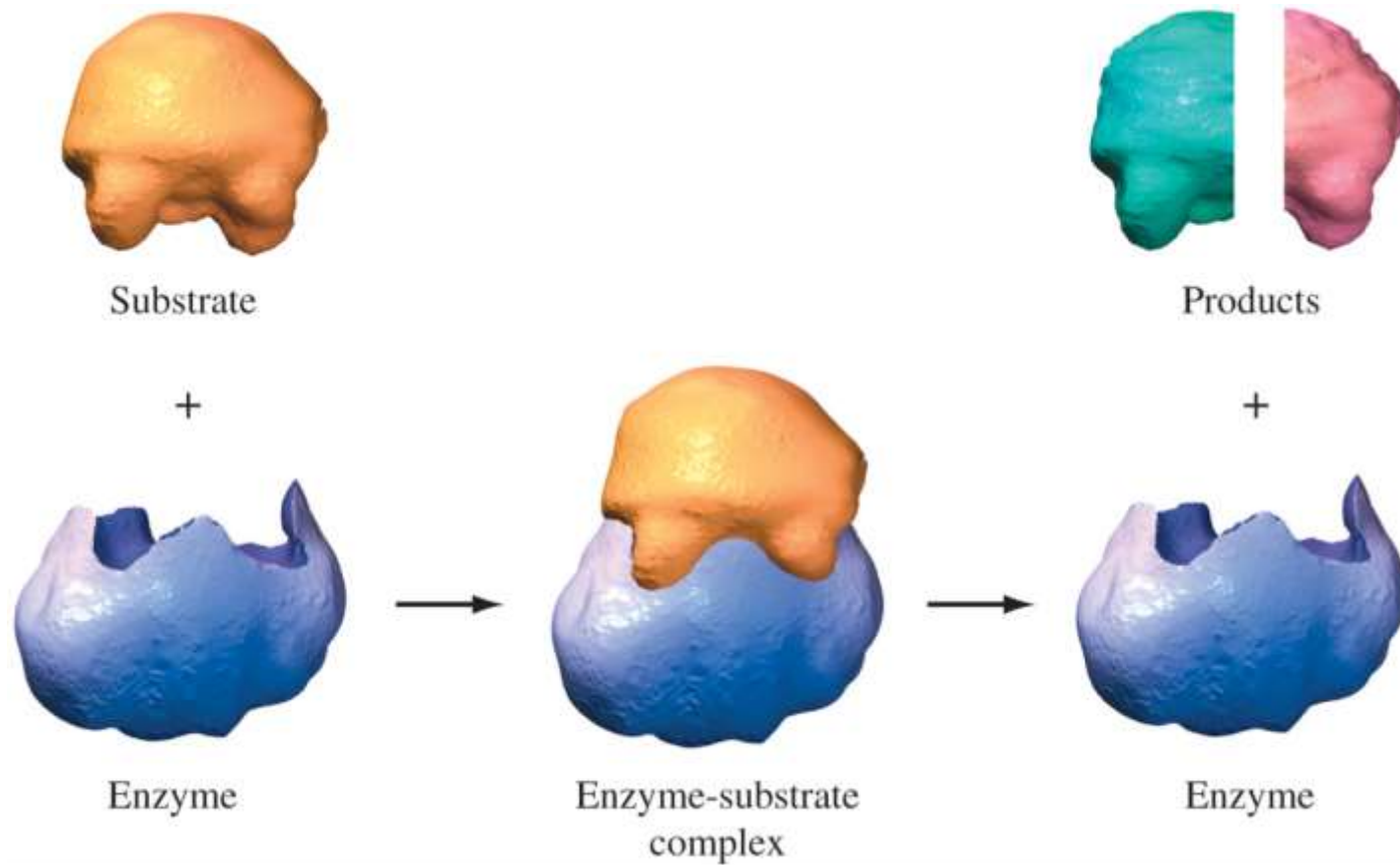


# Catalytic Converter



# Enzyme

Biological Catalyst







# **Reaction Energetics**

# Class Goals

- Understand the energy flow in a reaction
- To be able to calculate the energy needed for a reaction
- Understand Hess's Law

# Energy in Chemical Reactions

All chemical reactions involve bond 'rearrangements'. Bonds are broken and new ones are formed:

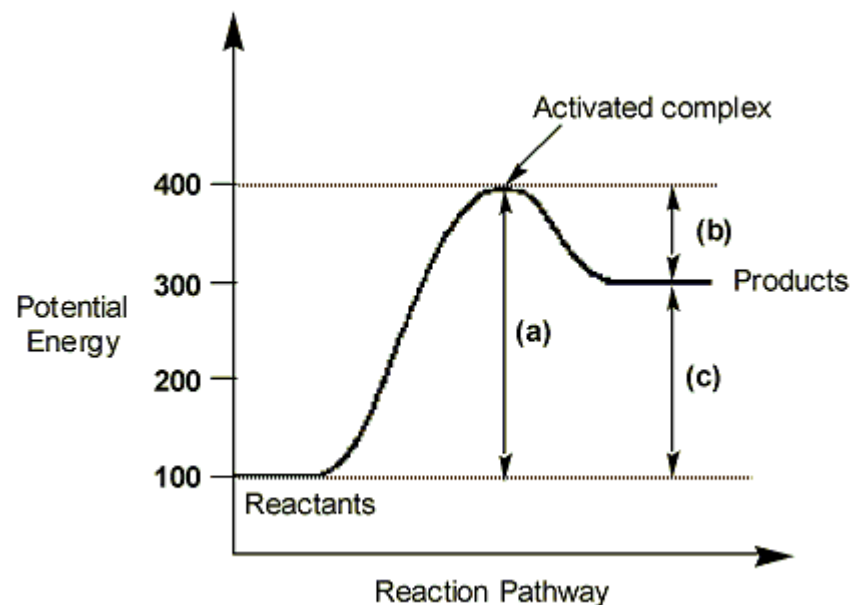
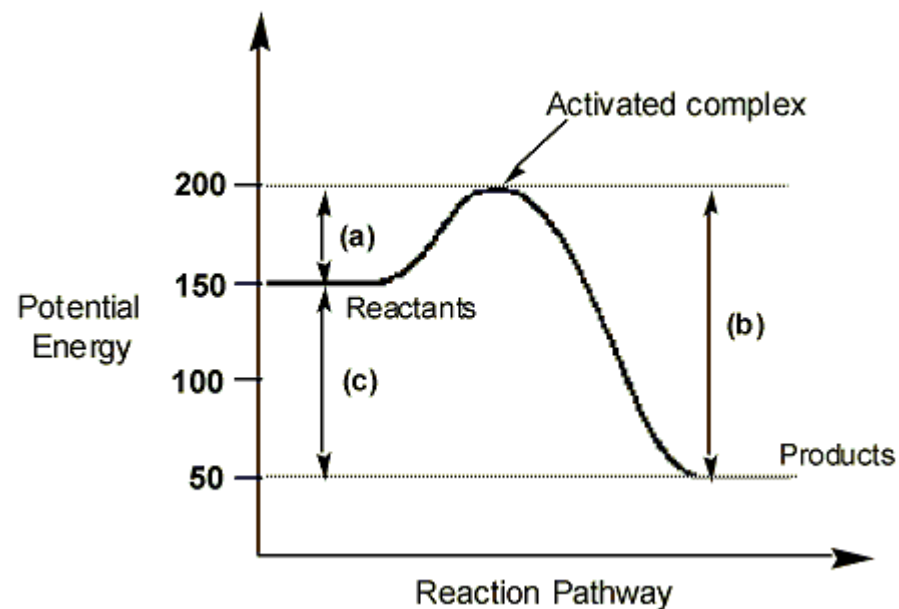
**Step 1:** Energy must be SUPPLIED to break chemical bonds of reactants

**Step 2:** Energy is RELEASED when new chemical bonds are made in the products

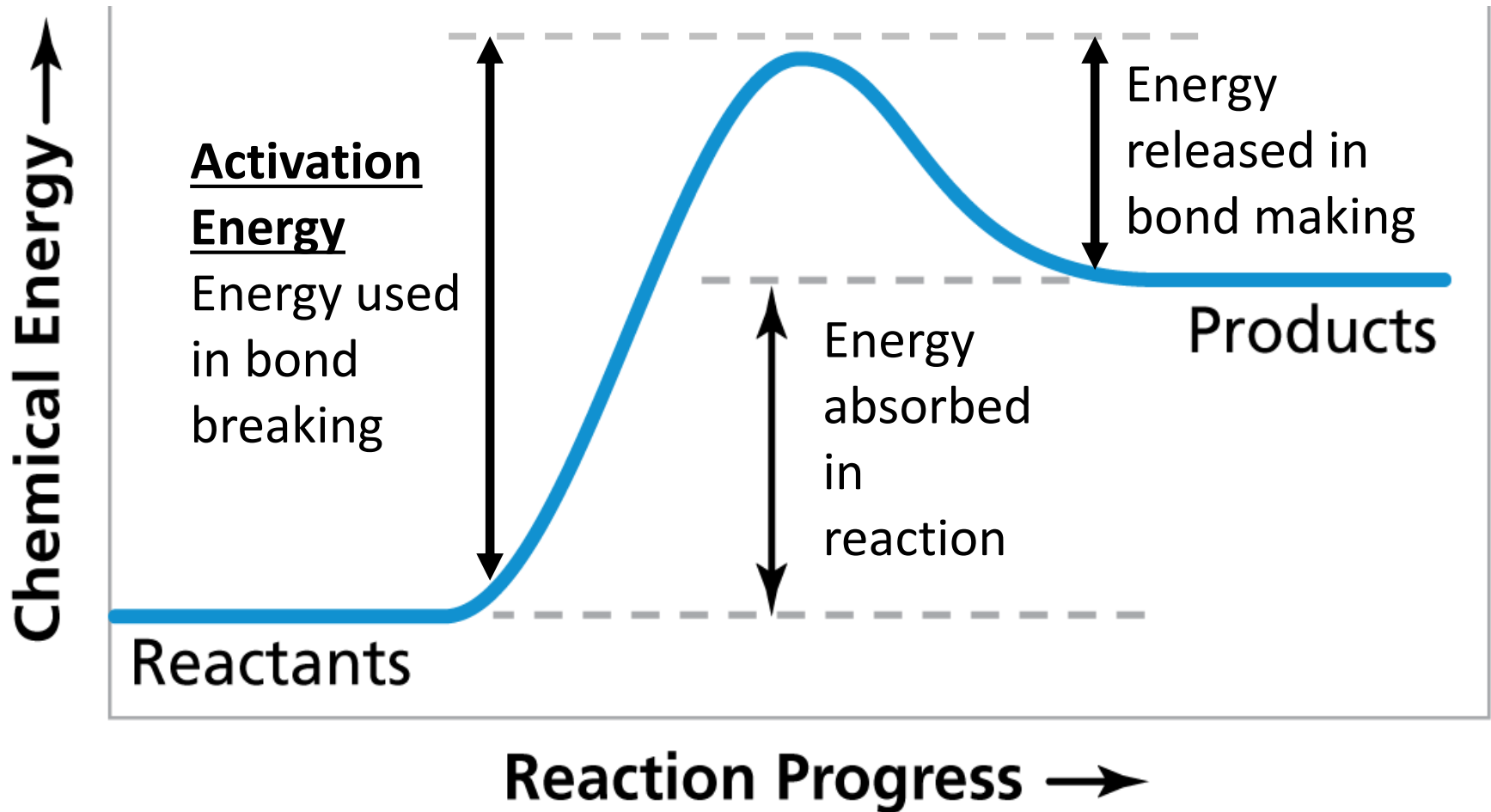
# Energy in Chemical Reactions

Breaking chemical bonds is always endothermic: is the Activation Energy!

Making chemical bonds is always exothermic.

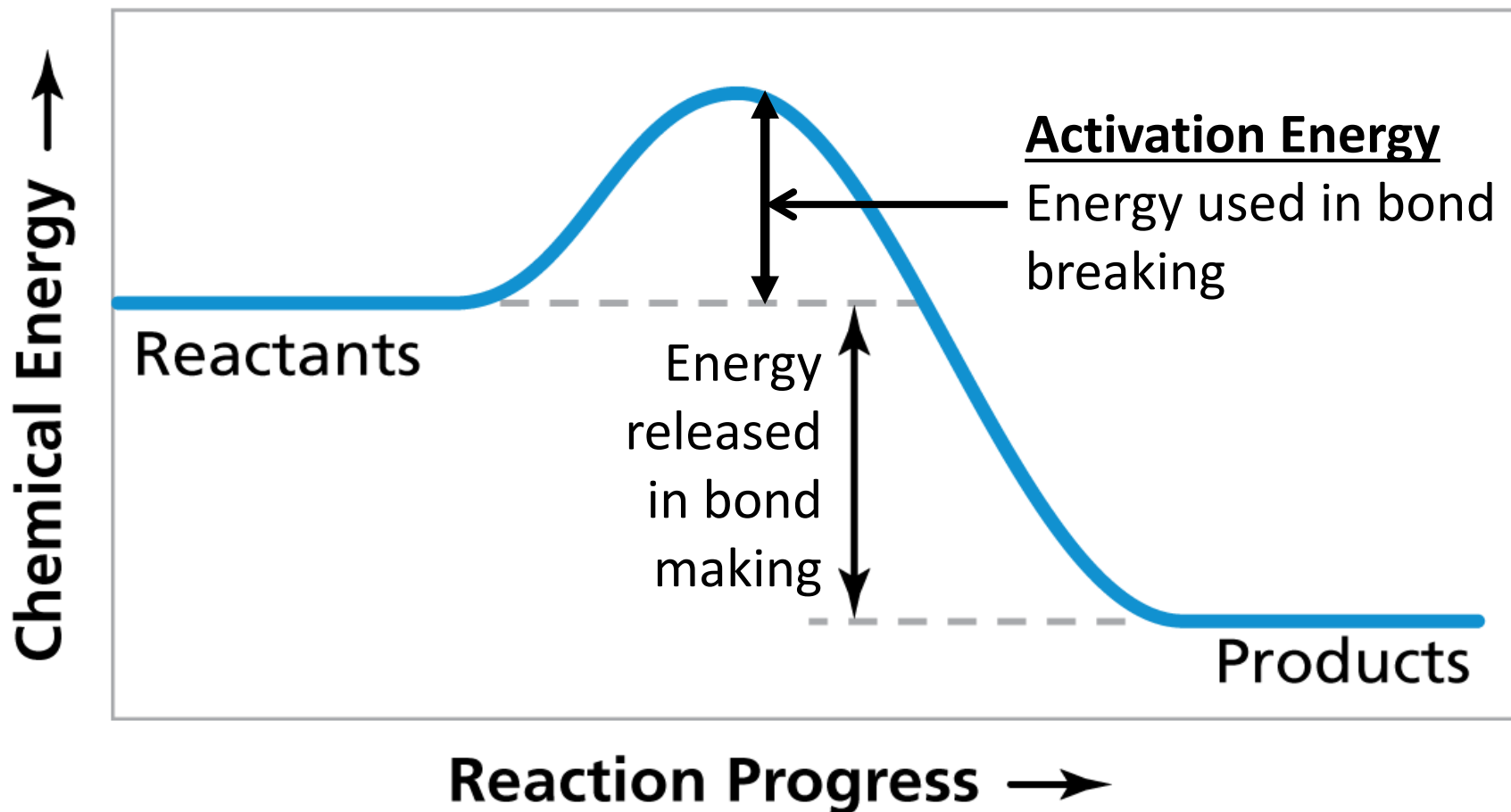


# Energy in Chemical Reactions



If more energy is ***SUPPLIED*** than is ***RELEASED*** then the reaction is ***ENDOTHERMIC***

# Energy in Chemical Reactions



A reaction is EXOTHERMIC if more energy is **RELEASED** than **SUPPLIED**.

# Thermodynamics

The area that study of energy, **energy transformations** and its relation to matter

**Enthalpy:** the sum of the internal energy of a system. A measure of the heat content at constant pressure.

You cannot measure the actual enthalpy of a substance, only an enthalpy **CHANGE**:  $\Delta H$

In a chemical reaction:

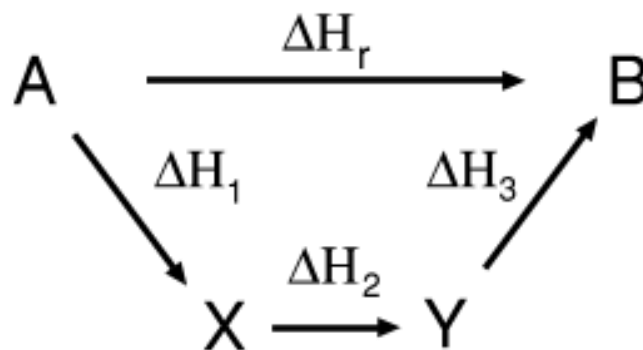
$$\Delta H = \text{Enthalpy of products} - \text{Enthalpy of reactants}$$

# HESS'S LAW

In a chemical reaction:

$$\Delta H = \text{Enthalpy of products} - \text{Enthalpy of reactants}$$

**“The enthalpy change is independent of the path taken”**



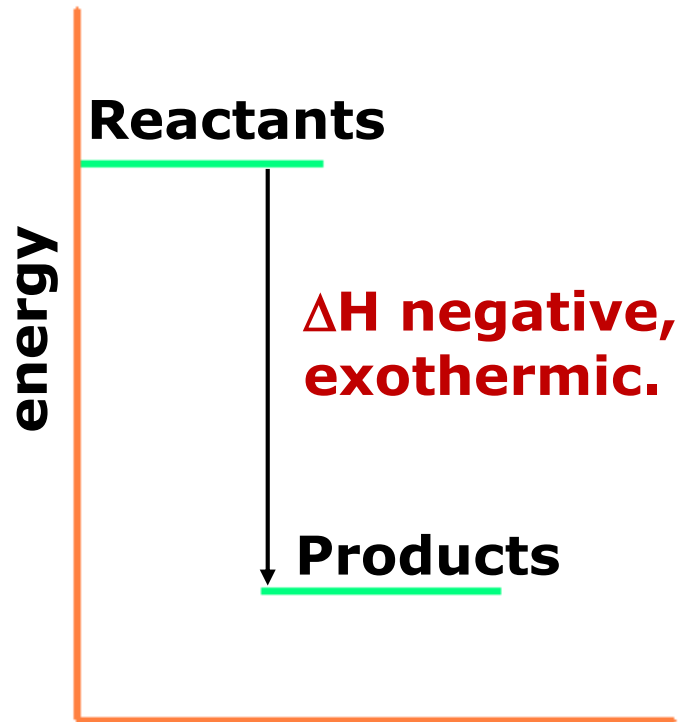
$$\Delta H_r = \Delta H_1 + \Delta H_2 + \Delta H_3$$

**Hess's Law:** When reactants are converted to products, the change in enthalpy is the same whether the reaction takes place in one step or in a series of steps.

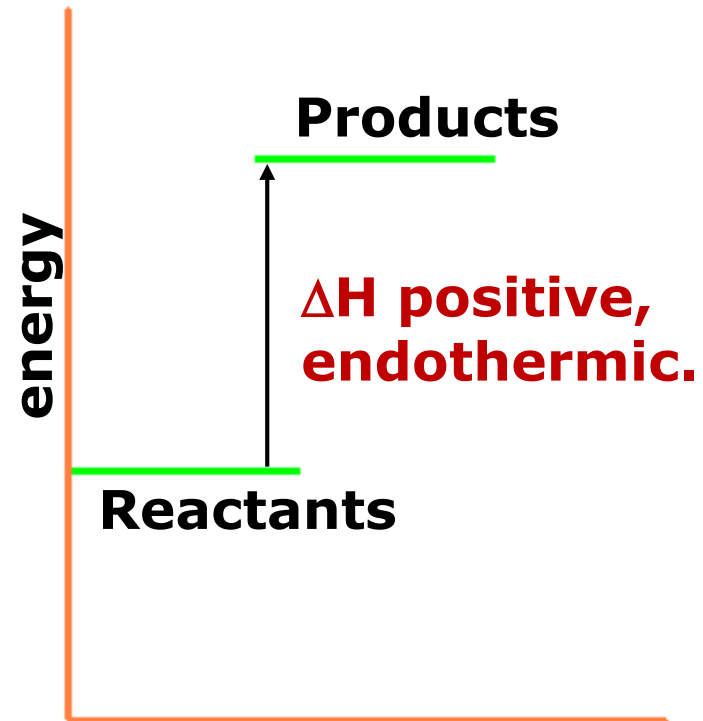


# Thermodynamics

This energy level diagram shows a reaction where  $\Delta H$  is negative (an exothermic reaction).



This energy level diagram shows a reaction where  $\Delta H$  is positive (an endothermic reaction).



# Thermodynamics

We will study 2 ways of how we can determine the total Enthalpy change in a Chemical reaction:

1. Using the **Enthalpy of bond dissociation**: we can discover the energy to build a specific molecule
2. Using the **Enthalpy of formation** of each reagent and product

# 1. Bond Dissociation Enthalpy

Energy required to break ONE MOLE of gaseous bonds to form gaseous atoms.

**Endothermic** - Energy must be put in to break any chemical bond



- strength of bonds depends on the phase of the material;
- **smaller bond enthalpy = weaker bond = easier to break**

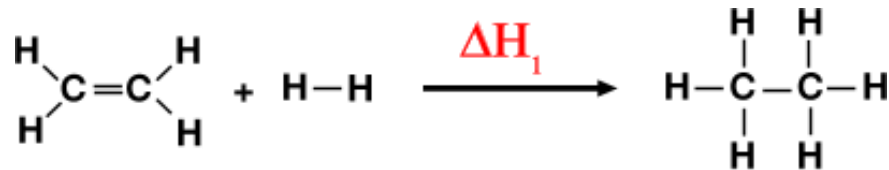
## Mean Values

H-H	436	H-F	562	N-N	163
C-C	346	H-C/	431	N=N	409
C=C	611	H-Br	366	N≡N	944
C≡C	837	H-I	299	P-P	172
C-O	360	H-N	388	F-F	158
C=O	743	H-O	463	C/C/	242
C-H	413	H-S	338	Br-Br	193
C-N	305	H-Si	318	I-I	151
C-F	484	P-H	322	S-S	264
C-C/	338	O-O	146	Si-Si	176

**UNITS = kJ mol<sup>-1</sup>**

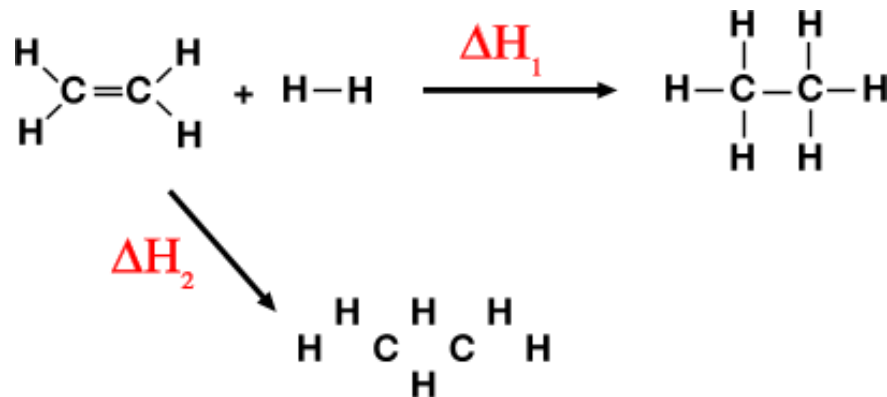
# 1. Enthalpy of reaction

Calculate the enthalpy change for the hydrogenation of ethene



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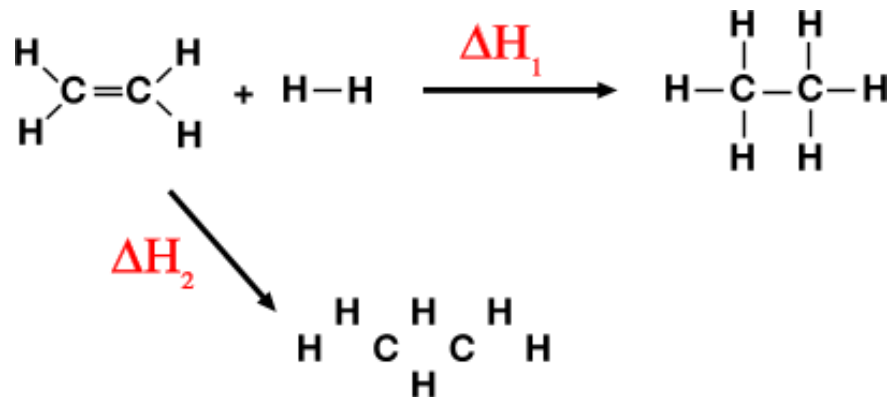
Calculate the enthalpy change for the hydrogenation of ethene



First step is breaking all the bonds in the reagent molecule (ethene)

# Enthalpy of reaction

Calculate the enthalpy change for the hydrogenation of ethene

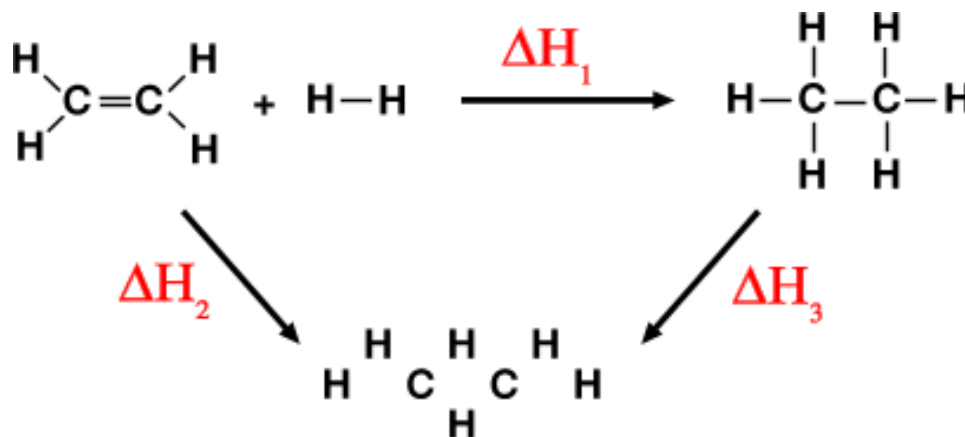


First step is breaking all the bonds in the reagent molecule (ethene)

$\Delta H_2$	1 x C=C bond	611 kJ/mol	=	611 kJ
	4 x C-H bonds	413 kJ/mol	=	1652 kJ
	1 x H-H bond	436 kJ/mol	=	436 kJ

**Total energy to break bonds of reactants = 2699 kJ**

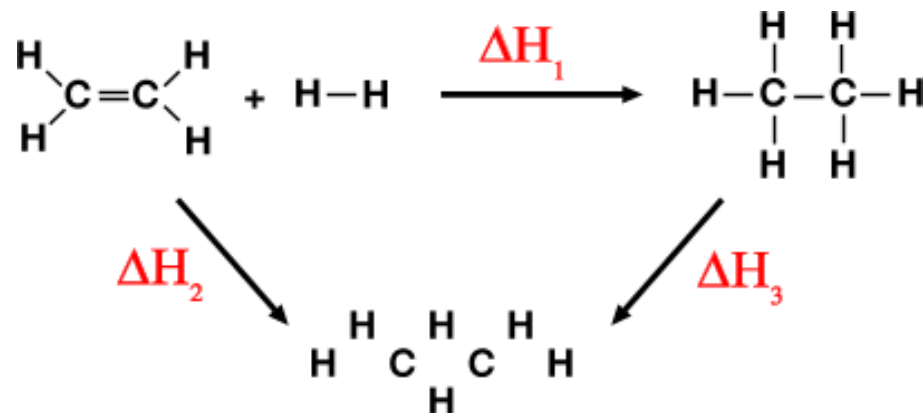
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**Second step is to calculate the energy in making the new bonds. The values are negative now !!**

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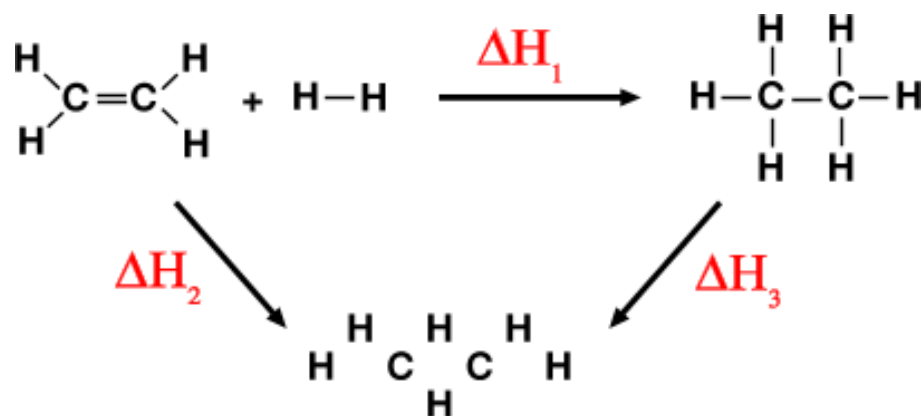
$\Delta H_3$	1 x C-C bond	-346 kJ/mol	=	-346 kJ
	6 x C-H bonds	-413 kJ/mol	=	-2478 kJ

**Total energy to break bonds of products = -2824 kJ**

$$2699 + (-2824) = -125 \text{ kJ}$$



# Enthalpy of reaction



Is this reaction  
Endothermic or  
Exothermic ?

**Total energy to break bonds of reactants = 2699 kJ**

Second step is to calculate the energy in making the new bonds. The values are negative now !!

$\Delta H_3$	1 x C-C bond	-346 kJ/mol	=	-346 kJ
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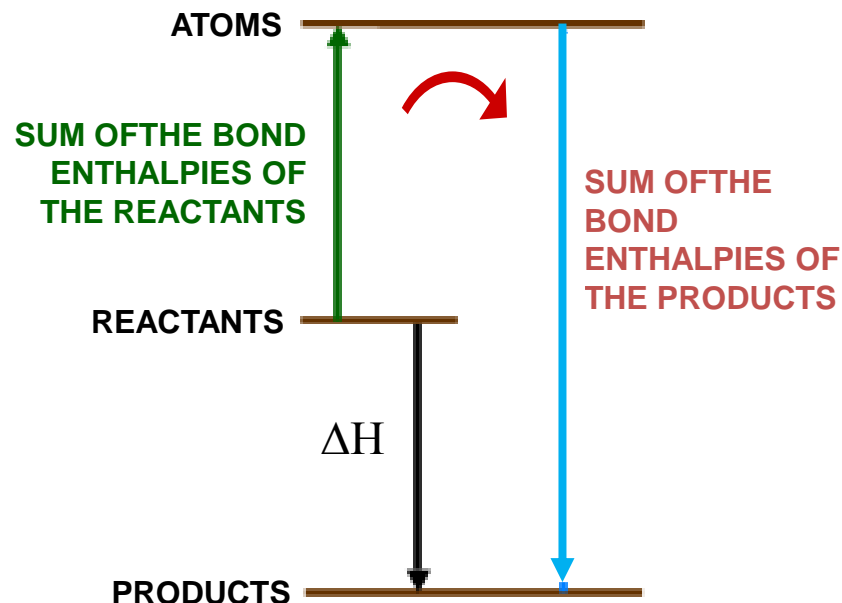
$$2699 + (-2824) = -125 \text{ kJ}$$

# Enthalpy of reaction

**Step 1** Energy is put in to break bonds to form separate, gaseous atoms.

**Step 2** Gaseous atoms then combine to form bonds and energy is released; its value will be equal and opposite to that of breaking the bonds

$$\Delta H_r = \text{Step 1} - \text{Step 2}$$



$$\Delta H = \Sigma \text{ bond enthalpies of reactants} - \Sigma \text{ bond enthalpies of products}$$

## 2. Standard Enthalpy of Formation

The enthalpy change when **ONE MOLE** of a compound is formed from its elements.

**Symbol:**  $\Delta_f H$  or  $\Delta H_f$

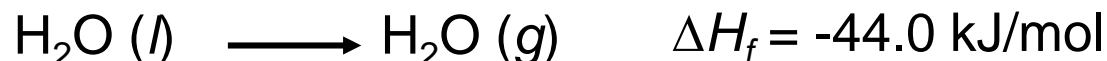
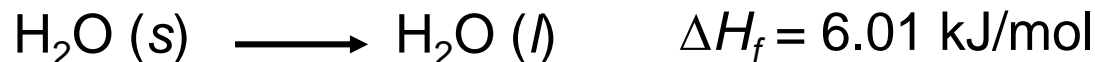
Only ONE MOLE of product in the equation

**Elements** in their standard states have **zero enthalpy of formation**.

Carbon is usually taken as the graphite allotrope.

$$\Delta H_f^0 (\text{C, graphite}) = 0$$

$$\Delta H_f^0 (\text{C, diamond}) = 1.90 \text{ kJ/mol}$$



## 2. Standard Enthalpy of Formation

- If you reverse a reaction, the sign of  $\Delta H$  changes



- If you multiply both sides of the equation by a factor  $n$ , then  $\Delta H$  must change by the same factor  $n$ .



- Remember that the phase state of the substance is important.

## 2. Enthalpy of Formation

Exercise:

How much heat is evolved when 266 g of white phosphorus ( $P_4$ ) burn in air?



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Remember, the Enthalpy of formation is described for 1 mol of product

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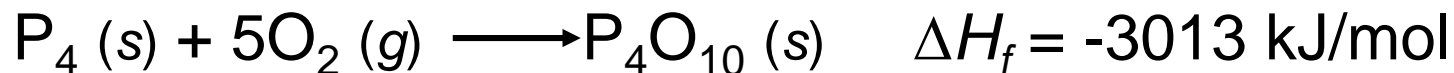


$$266 \text{ g } P_4 \times \frac{1 \text{ mol } P_4}{123.9 \text{ g } P_4} = 2.15 \text{ mol}$$

## 2. Enthalpy of Formation

Exercise:

How much heat is evolved when 266 g of white phosphorus ( $P_4$ ) burn in air?



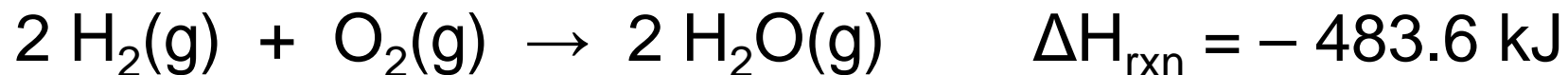
$$266 \text{ g } P_4 \times \frac{1 \text{ mol } P_4}{123.9 \text{ g } P_4} = 2.15 \text{ mol}$$

$$2.15 \text{ mol} \times 3013 \text{ kJ/mol} = 6470 \text{ kJ}$$



## 2. Enthalpy of Formation

What is the enthalpy change when 178 g of  $\text{H}_2\text{O}_{(\text{g})}$  are produced?

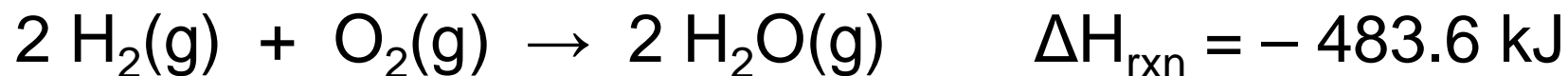


The space shuttle was powered by the reaction above !



## 2. Enthalpy of Formation

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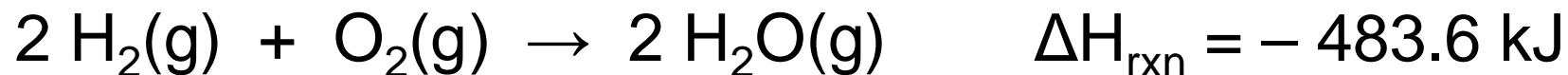


This is the reaction Enthalpy, so it is the total change for this reaction  $\rightarrow$  2 mol of products!



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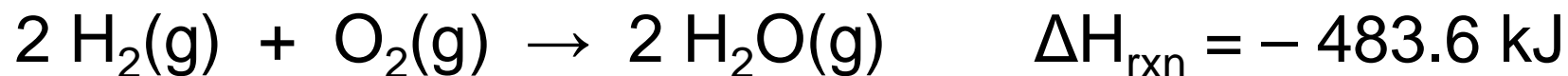
This is the reaction Enthalpy, so it is the total change for this reaction  $\rightarrow$  2 mol of products!

I need to divide  $\Delta H_{\text{rxn}}$  by 2 to have the  $\Delta H_{\text{f}}$ .



## 2. Enthalpy of Formation

What is the enthalpy change when 178 g of  $\text{H}_2\text{O}_{(\text{g})}$  are produced?



$$178 \text{ g H}_2\text{O} \times \frac{1 \text{ mol H}_2\text{O}}{18 \text{ g}} = 9.88 \text{ mol}$$

$$9.88 \text{ mol} \times -241.8 \text{ kJ/mol} = 2391.1 \text{ kJ}$$



## 2. Enthalpy of Reaction

Calculate the standard enthalpy change for the following reaction, given that the standard enthalpies of formation of water, nitrogen dioxide and nitric acid are  $-286$ ,  $+33$  and  $-173 \text{ kJ mol}^{-1}$  respectively;



## 2. Enthalpy of Reaction

Calculate the standard enthalpy change for the following reaction, given that the standard enthalpies of formation of water, nitrogen dioxide and nitric acid are  $-286$ ,  $+33$  and  $-173 \text{ kJ mol}^{-1}$  respectively;



$$\Delta H = \Sigma \Delta_f H \text{ of products} - \Sigma \Delta_f H \text{ of reactants}$$

## 2. Enthalpy of Reaction

Calculate the standard enthalpy change for the following reaction, given that the standard enthalpies of formation of water, nitrogen dioxide and nitric acid are  $-286$ ,  $+33$  and  $-173 \text{ kJ mol}^{-1}$  respectively;



$$\Delta H = \Sigma \Delta_f H \text{ of products} - \Sigma \Delta_f H \text{ of reactants}$$

the value for oxygen is ZERO as it is an element!

## 2. Enthalpy of Reaction

Calculate the standard enthalpy change for the following reaction, given that the standard enthalpies of formation of water, nitrogen dioxide and nitric acid are  $-286$ ,  $+33$  and  $-173 \text{ kJ mol}^{-1}$  respectively;



$$\Delta H = \Sigma \Delta_f H \text{ of products} - \Sigma \Delta_f H \text{ of reactants}$$

**PRODUCTS**

$$[ 4 \times \Delta_f H \text{ of HNO}_3 ]$$

**REACTANTS**

$$- [ (2 \times \Delta_f H \text{ of H}_2\text{O}) + (4 \times \Delta_f H \text{ of NO}_2) + (1 \times \Delta_f H \text{ of O}_2) ]$$



## 2. Enthalpy of Reaction

Calculate the standard enthalpy change for the following reaction, given that the standard enthalpies of formation of water, nitrogen dioxide and nitric acid are  $-286$ ,  $+33$  and  $-173 \text{ kJ mol}^{-1}$  respectively;



$$\Delta H = \Sigma \Delta_f H \text{ of products} - \Sigma \Delta_f H \text{ of reactants}$$

**PRODUCTS**

$$[ 4 \times \Delta_f H \text{ of HNO}_3 ] - [ (2 \times \Delta_f H \text{ of H}_2\text{O}) + (4 \times \Delta_f H \text{ of NO}_2) + (1 \times \Delta_f H \text{ of O}_2) ]$$

**REACTANTS**

$$\Delta H^\circ_{\text{rxn}} = 4 \times (-173) - 2 \times (-286) + 4 \times (+33) + 0$$

$$\text{ANSWER} = -252 \text{ kJ}$$

# Be careful !

When using the Bond Enthalpies, the formula for the  $\Delta H$  is:

$$\Delta H = \Sigma \text{ bond enthalpies of reactants} - \Sigma \text{ bond enthalpies of products}$$

However, when using the Enthalpies of Formation, the formula for the  $\Delta H$  is:

$$\Delta H = \Sigma \Delta_f H \text{ of products} - \Sigma \Delta_f H \text{ of reactants}$$

## 2. Enthalpy of Reaction

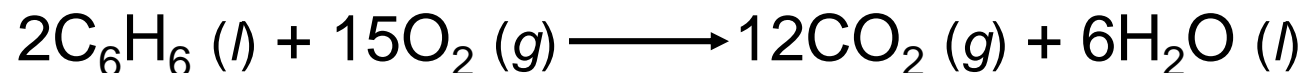
Calculate the standard enthalpy of formation of methane; the standard enthalpies of formation of hydrogen and methane are -286 and -890 kJ mol<sup>-1</sup> .



YOU !

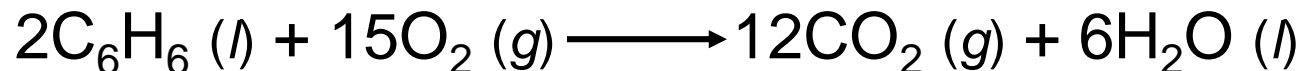
## 2. Enthalpy of Reaction

How much heat is released per mole of benzene ( $\text{C}_6\text{H}_6$ ) combusted? The standard enthalpy of formation of benzene is 49.04 kJ/mol,  $\text{CO}_2$  is  $-393.5$  kJ/mol;  $\text{H}_2\text{O}$  is  $-187.6$  kJ/mol.



## 2. Enthalpy of Reaction

How much heat is released per mole of benzene ( $\text{C}_6\text{H}_6$ ) combusted? The standard enthalpy of formation of benzene is 49.04 kJ/mol,  $\text{CO}_2$  is -393.5 kJ/mol;  $\text{H}_2\text{O}$  is -187.6 kJ/mol.



$$\Delta H_{\text{rxn}} = [ 12\Delta H_{\text{f}}(\text{CO}_2) + 6\Delta H_{\text{f}}(\text{H}_2\text{O}) ] - [ 2\Delta H_{\text{f}}(\text{C}_6\text{H}_6) ]$$

$$\Delta H_{\text{rxn}} = [ 12 \times -393.5 + 6 \times -187.6 ] - [ 2 \times 49.04 ] = -5946 \text{ kJ}$$

$$\frac{-5946 \text{ kJ}}{2 \text{ mol}} = -2973 \text{ kJ/mol C}_6\text{H}_6$$

## 2. Enthalpy of Reaction

What is the  $\Delta H_{\text{rxn}}$  for the complete combustion of Butane,  $\text{C}_4\text{H}_{10}$  ?  $\text{CO}_2$  is  $-393.5 \text{ kJ/mol}$ ;  $\text{H}_2\text{O}$  is  $-187.6 \text{ kJ/mol}$ ,  $\text{C}_4\text{H}_{10}$  is  $-124.7 \text{ kJ/mol}$

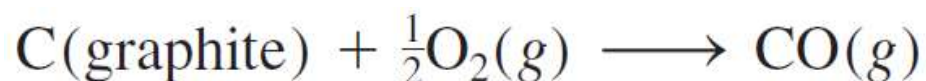


YOU !

## 2. Enthalpy of Reaction

Hess's law can be applied to find the reaction Enthalpy by combining the Enthalpy of other reactions !

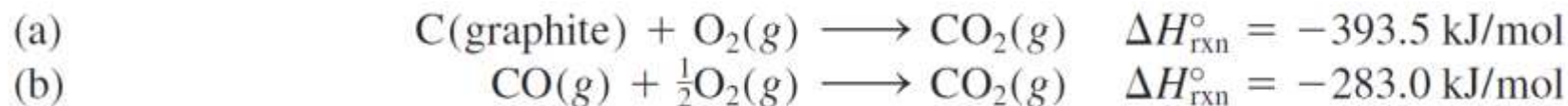
Let's say we are interested in the standard enthalpy of formation of carbon monoxide (CO).



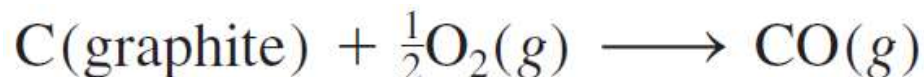
However, burning graphite also produces some carbon dioxide (CO<sub>2</sub>), so we cannot measure the enthalpy change for CO directly.

We must employ an indirect route, based on Hess's law.

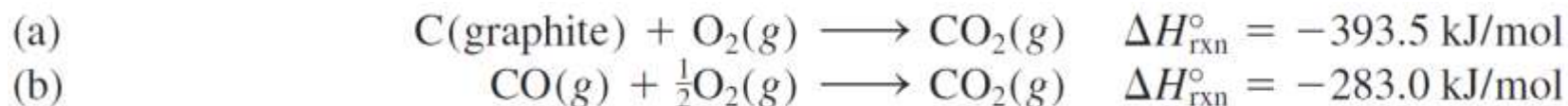
It is possible to carry out the following two separate reactions:



## 2. Enthalpy of Reaction

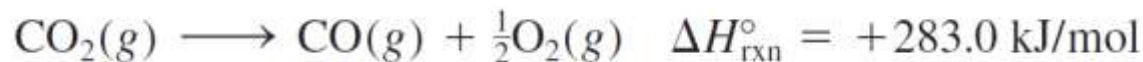


I have the two following separate reactions:



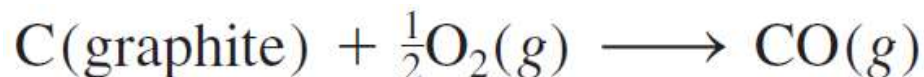
First, I have to organize the reactions in order to have my desired reagents on left and the products on the right.

In this case, we need to reverse Equation (b):

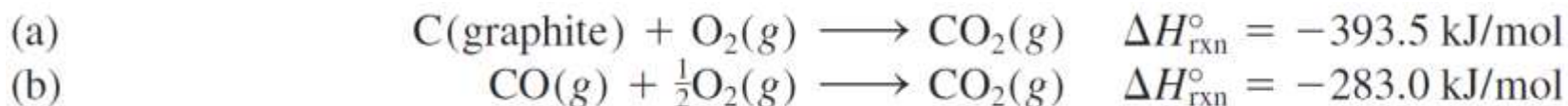




## 2. Enthalpy of Reaction

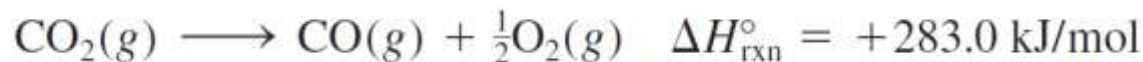


I have the two following separate reactions:



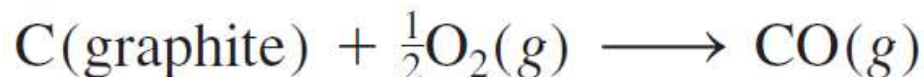
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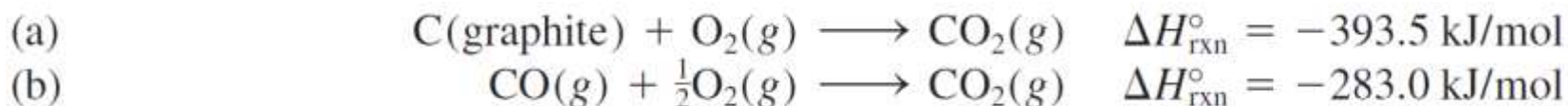


Remember to change the signal of the  $\Delta H$  !

### 3. Enthalpy of Reaction

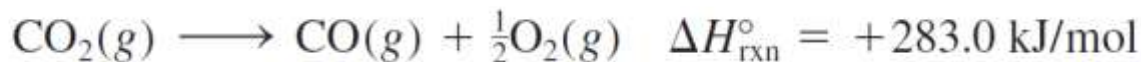


I have the two following separate reactions:

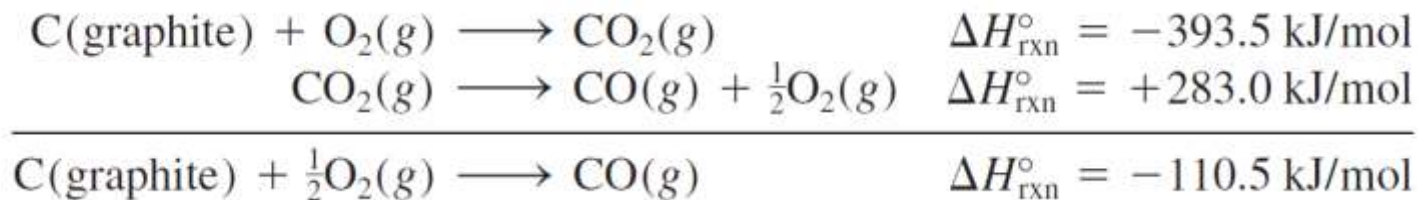


First, I have to organize the reactions in order to have my desired reagents on left and the products on the right.

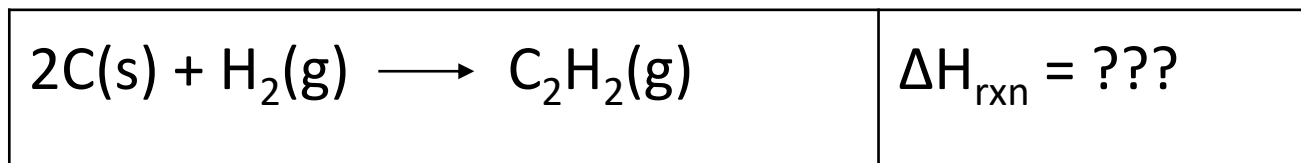
In this case, we need to reverse Equation (b):



Now make the sum



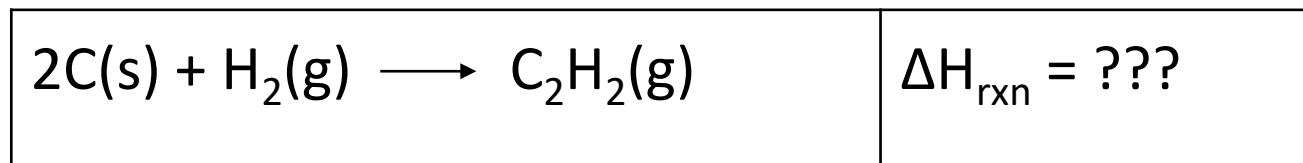
### 3. Enthalpy of Reaction



You have the following thermochemical equations:

$\text{C}_2\text{H}_2\text{(g)} + (5/2)\text{O}_2\text{(g)} \longrightarrow 2\text{CO}_2\text{(g)} + \text{H}_2\text{O(l)}$	$\Delta H^\circ = -1299.5 \text{ kJ}$
$\text{C(s)} + \text{O}_2\text{(g)} \longrightarrow \text{CO}_2\text{(g)}$	$\Delta H^\circ = -393.5 \text{ kJ}$
$\text{H}_2\text{(g)} + (1/2)\text{O}_2\text{(g)} \longrightarrow \text{H}_2\text{O(l)}$	$\Delta H^\circ = -285.8 \text{ kJ}$

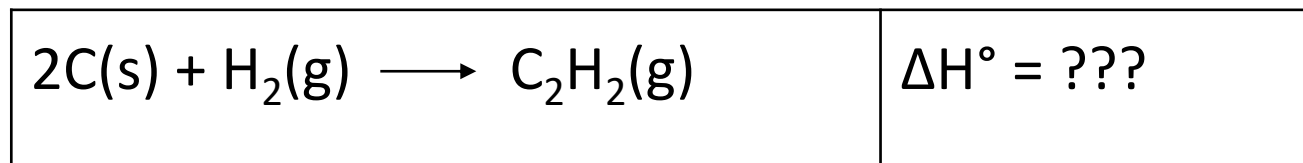
### 3. Enthalpy of Reaction



You have the following thermochemical equations:

$\text{C}_2\text{H}_2\text{(g)} + (5/2)\text{O}_2\text{(g)} \longrightarrow 2\text{CO}_2\text{(g)} + \text{H}_2\text{O(l)}$	$\Delta H^\circ = -1299.5 \text{ kJ}$
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$\text{H}_2\text{(g)} + (1/2)\text{O}_2\text{(g)} \longrightarrow \text{H}_2\text{O(l)}$	$\Delta H^\circ = -285.8 \text{ kJ}$

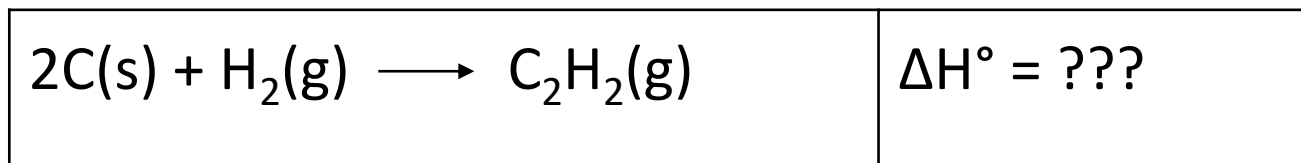
### 3. Enthalpy of Reaction



You have the following thermochemical equations:

$2\text{CO}_2\text{(g)} + \text{H}_2\text{O(l)} \longrightarrow \text{C}_2\text{H}_2\text{(g)} + (5/2)\text{O}_2\text{(g)}$	$\Delta\text{H}^\circ = +1299.5 \text{ kJ}$
$\text{C(s)} + \text{O}_2\text{(g)} \longrightarrow \text{CO}_2\text{(g)}$	$\Delta\text{H}^\circ = -393.5 \text{ kJ}$
$\text{H}_2\text{(g)} + (1/2)\text{O}_2\text{(g)} \longrightarrow \text{H}_2\text{O(l)}$	$\Delta\text{H}^\circ = -285.8 \text{ kJ}$

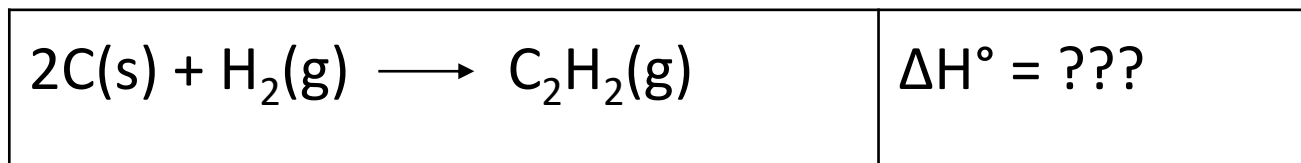
### 3. Enthalpy of Reaction



You have the following thermochemical equations:

$2\text{CO}_2\text{(g)} + \text{H}_2\text{O(l)} \longrightarrow \text{C}_2\text{H}_2\text{(g)} + (5/2)\text{O}_2\text{(g)}$	$\Delta\text{H}^\circ = +1299.5 \text{ kJ}$
$\text{C(s)} + \text{O}_2\text{(g)} \longrightarrow \text{CO}_2\text{(g)}$	$\Delta\text{H}^\circ = -393.5 \text{ kJ}$
$\text{H}_2\text{(g)} + (1/2)\text{O}_2\text{(g)} \longrightarrow \text{H}_2\text{O(l)}$	$\Delta\text{H}^\circ = -285.8 \text{ kJ}$

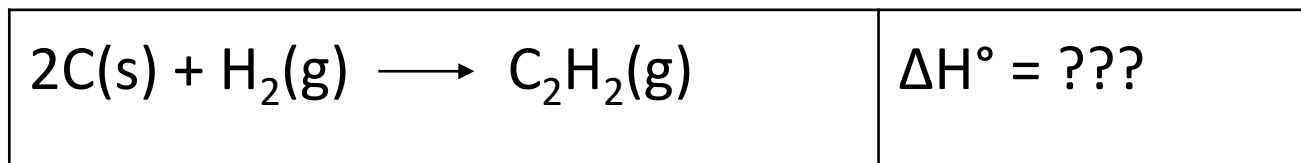
### 3. Enthalpy of Reaction



You have the following thermochemical equations:

$2\text{CO}_2\text{(g)} + \text{H}_2\text{O(l)} \longrightarrow \text{C}_2\text{H}_2\text{(g)} + (5/2)\text{O}_2\text{(g)}$	$\Delta\text{H}^\circ = +1299.5 \text{ kJ}$
$2\text{C(s)} + 2\text{O}_2\text{(g)} \longrightarrow 2\text{CO}_2\text{(g)}$	$\Delta\text{H}^\circ = 2\text{X} (-393.5) \text{ kJ}$
$\text{H}_2\text{(g)} + (1/2)\text{O}_2\text{(g)} \longrightarrow \text{H}_2\text{O(l)}$	$\Delta\text{H}^\circ = -285.8 \text{ kJ}$

### 3. Enthalpy of Reaction

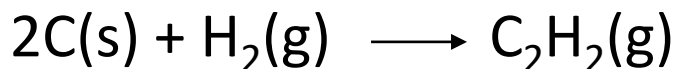


You have the following thermochemical equations:

$2\text{CO}_2\text{(g)} + \text{H}_2\text{O(l)} \longrightarrow \text{C}_2\text{H}_2\text{(g)} + (5/2)\text{O}_2\text{(g)}$	$\Delta\text{H}^\circ = +1299.5 \text{ kJ}$
$2\text{C(s)} + 2\text{O}_2\text{(g)} \longrightarrow 2\text{CO}_2\text{(g)}$	$\Delta\text{H}^\circ = 2\text{X} (-393.5) \text{ kJ}$
$\text{H}_2\text{(g)} + (1/2)\text{O}_2\text{(g)} \longrightarrow \text{H}_2\text{O(l)}$	$\Delta\text{H}^\circ = -285.8 \text{ kJ}$



### 3. Enthalpy of Reaction



$$\Delta H^\circ = ???$$

$2\text{CO}_2\text{(g)} + \text{H}_2\text{O(l)} \longrightarrow \text{C}_2\text{H}_2\text{(g)} + (5/2)\text{O}_2\text{(g)}$	$\Delta H^\circ = +1299.5 \text{ kJ}$
$2\text{C(s)} + 2\text{O}_2\text{(g)} \longrightarrow 2\text{CO}_2\text{(g)}$	$\Delta H^\circ = 2X (-393.5) \text{ kJ}$
$\text{H}_2\text{(g)} + (1/2)\text{O}_2\text{(g)} \longrightarrow \text{H}_2\text{O(l)}$	$\Delta H^\circ = -285.8 \text{ kJ}$

1. Control that you have the right reaction by summing the reagents and products
2. Adding everything:  $+1299.5 \text{ kJ} + (-787 \text{ kJ}) + (-285.8 \text{ kJ}) = \mathbf{+226.7 \text{ kJ}}$

# Standard Enthalpy Changes

Why a

**standard?** Enthalpy values vary according to the conditions

**Pressure:** **100 kPa (1 atmosphere)**

**A stated temperature** **298K (25°C)**

- assign the correct subscript [(g), (l) or (s)] to indicate which state
- any solutions are of concentration 1 M
- if is standard conditions, the symbol for  $\Delta H$  is modified.

$\Delta H$

$\Delta H^{\ominus}_{298}$

Enthalpy Change

Standard Enthalpy Change  
(at 298K)