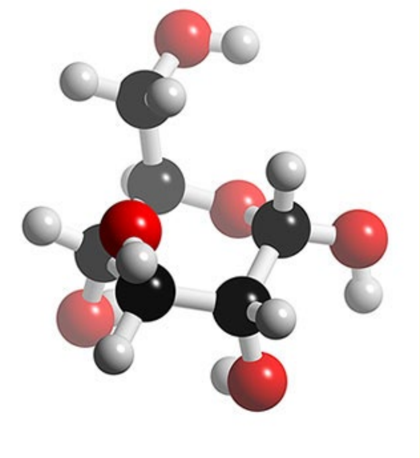
Thermochemistry

A. Energy

- ✶we use hydrocarbons in many areas of our lives

eg) **glucose for cellular respiration**



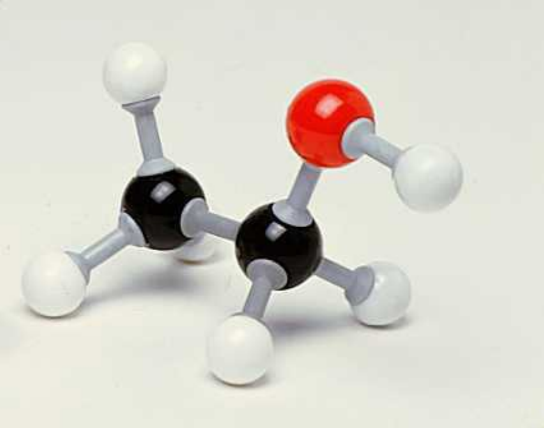
gasoline and natural gas for fuel

- the energy stored in the chemical bonds of hydrocarbons originally comes from the **sun**

- ancient plants captured the energy of the sun during **photosynthesis**, ancient animals ate the plants, then death and trapping in rock formations as oil, gas, oil sand etc.

✶there are two fundamental types of energy:

1. **kinetic energy (E_K):** the energy of **motion** (of particles)



2. **potential energy (E_P):** energy that is **stored** (in chemical bonds)

✶ the First Law of Thermodynamics states that:

- the total energy of the universe is **constant**
- energy can be **converted to other forms** however the **total energy** of any system is **conserved** (it **cannot** be created or destroyed)

- the Second Law of Thermodynamics states that:
  - in the absence of energy input, a system becomes more **disordered**
  - heat will always transfer from **hot objects to cooler objects** until **thermal equilibrium** is reached

B. Temperature Change

- **temperature** is a measure of the **average kinetic energy** of the particles of a substance

- the **faster** the particles are moving, the **higher** the temperature

- the amount of energy needed to heat a substance depends on three factors:

    1. the **mass** of the substance
    2. the **change in temperature**
    3. the **type** of substance (heat capacity)

- heat capacity is heat required to change the temperature of **one gram** of a substance by **1°C**

$$\boxed{\mathbf{Q = mc\Delta t}}$$

where: Q = heat energy in J
m = mass in g
Δt = change in temperature in °C
c = specific heat capacity in J/g°C

Example

Find the heat required to change 2.50 g of water from 10.0°C to 27.0°C .

$$\begin{aligned} Q &= mc\Delta t \\ &= (2.50\ \text{g})(4.19\ \text{J/g°C})\ (27.0\text{°C} - 10.0\ \text{°C}) \\ &= 178.075\ \text{J} \\ &= \mathbf{178\ J} \end{aligned}$$

C. Energy and Enthalpy

- **enthalpy** is the sum of all forms of kinetic and potential energy in a system ($E_K + E_P$)
- unfortunately, the enthalpy of individual substances cannot be measured directly (E_K can with a thermometer but how do you measure E_P?)
- changes in enthalpy occur whenever heat is **released or absorbed in a physical, chemical or nuclear change…** fortunately, this can be measured

- **enthalpy change, ΔH,** is measured in **J or kJ**
- subscripts are sometimes used to denote the type of process, for example “r” for “reaction”

$\mathbf{\Delta_r H}$ = enthalpy of reaction

- the “°” symbol is used to denote changes taking place at **standard** conditions

$\mathbf{\Delta_r H^\circ}$ = standard enthalpy of reaction (at SATP 100 kPa and 25°C)

- **molar enthalpy** is the enthalpy change **per mole** of a substance
- molar enthalpy is also designated as ΔH, although we will be using just **H** for our formulas
- molar enthalpy is measured in **J/mol or kJ/mol**

***this can be confusing so pay close attention to the context…wording and units!!!

D. Energy Change in Chemical Reactions

- changes in **potential energy** take place during chemical reactions when one substance is **converted into another substance**
- chemical bonds are sources of **stored** potential energy
- **breaking** bonds **requires** energy
- **forming** bonds **releases** energy

- if the energy added to break the bonds is **greater** than the energy released when the new bonds are formed then the reaction is **endothermic**

eg) **photosynthesis**

$$6\,CO_2(g) + 6\,H_2O(l) + \text{energy} \rightarrow C_6H_{12}O_6(s) + 6\,O_2(g)$$

monster flower

- endothermic changes are designated as **positive values** since energy is being **added** to the system

- if the energy added to break the bonds is **less** than the energy released when the new bonds are formed then the reaction is **exothermic**

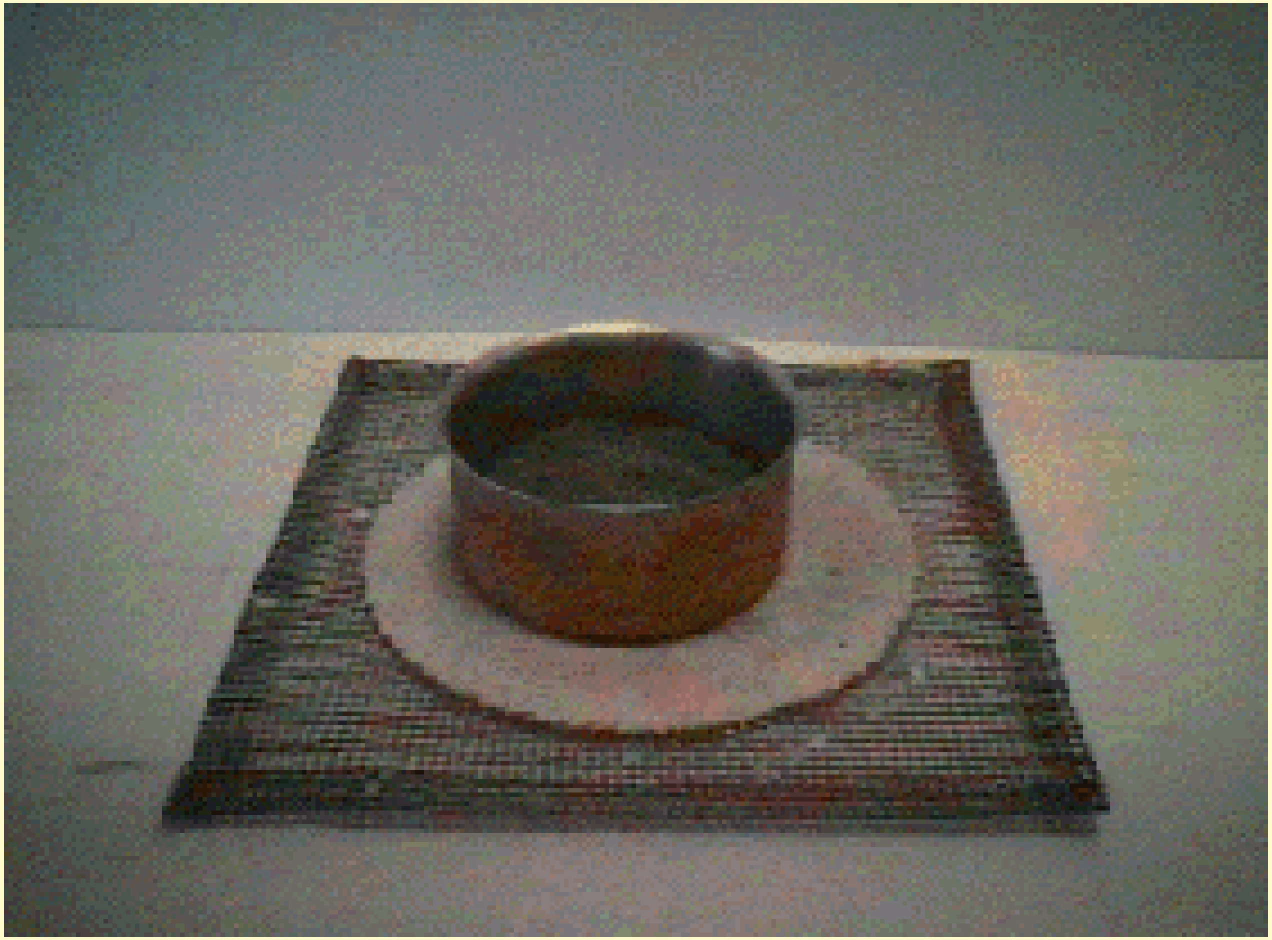
eg) **cellular respiration**

$$C_6H_{12}O_6(s) + 6\,O_2(g) \rightarrow 6\,CO_2(g) + 6\,H_2O(l) + \text{energy}$$

eg) **hydrocarbon combustion**

hydrocarbon + $O_2(g)$ → $CO_2(g)$ + $H_2O(g)$ + energy

- exothermic changes are designated as **negative values** since energy is being **removed** from the system



- the amount of energy lost or gained is **directly proportional** to the amount of substances that react

  ie) if 100 g of a substance burning will release **twice as much** energy compared to when 50 g of that same substance burns

E. Communicating Enthalpy Changes

Exothermic Reactions

1. $\Delta_r H$ Notation

- ★ the heat of reaction can be given as a $\Delta_r H$ value **outside** of the equation
- ★ the sign on $\Delta_r H$ is **negative** since the enthalpy of the system is **decreasing**

$$2\,SO_2(g) + O_2(g) \rightarrow 2\,SO_3(g) \qquad \Delta_r H = -197.8\ kJ$$

2. Inside the Equation

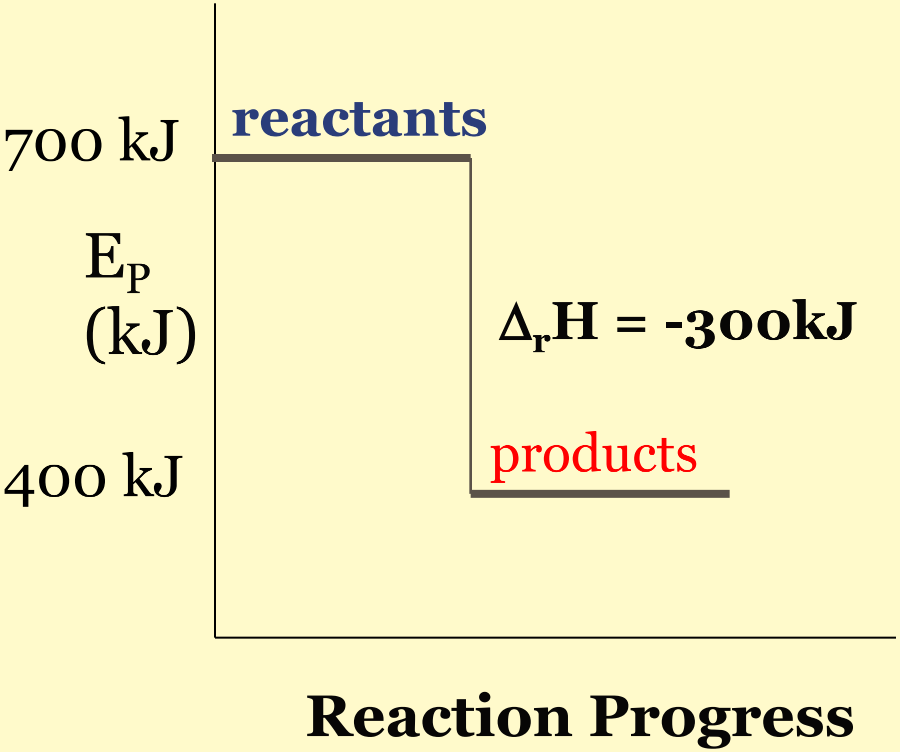
- in an exothermic reaction enthalpy is included as a **product**

$$\mathbf{Mg(s) + \tfrac{1}{2}\,O_2(g) \rightarrow MgO(s) + 601.6\ kJ}$$

3. Potential Energy Diagrams

- shows the potential energy of the **reactants** and the **products** of a chemical reaction
- reactants have **more** potential energy than the products in an exothermic reaction
- the difference between the reactants and products is the $\mathbf{\Delta_r H}$

Exothermic



Products have **less** E_p than the reactants ∴ energy has been **lost** to the surroundings

$$\text{Reactants} = \text{Products} + \Delta_r H$$

Endothermic Reactions

1. Δ_rH Notation

- the sign on ΔrH is **positive** since the enthalpy of the system is **increasing**

$$\mathbf{2\,SO_{3(}g) \rightarrow 2\,SO_2(g) + O_2(g) \qquad \Delta_r H = +197.8\ kJ}$$

2. Inside the Equation

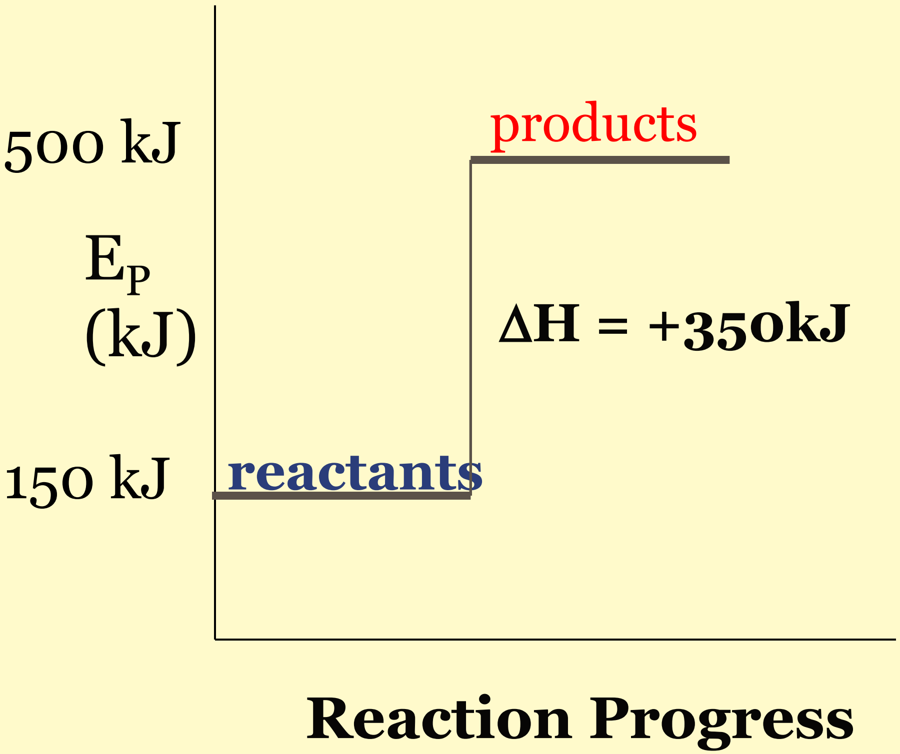
- in an endothermic reaction enthalpy is included as a **reactant**

$$\mathbf{H_2O(l) + 285.8\ kJ \rightarrow H_2(g) + \tfrac{1}{2}\,O_2(g)}$$

3. Potential Energy Diagrams

- reactants have **less** potential energy than the products in an exothermic reaction
- the difference between the reactants and products is the $\Delta_r H$

Endothermic



500 kJ

E_P (kJ)

products

ΔH = +350kJ

150 kJ

reactants

Reaction Progress

Products have **more** E_p than the reactants ∴ energy has been **gained** by the system

Reactants + $\Delta_r H$ = Products

- cellular respiration is a low temperature combustion of the hydrocarbon glucose, producing **$CO_2(g)$** and **$H_2O(l)$**

$$C_6H_{12}O_6(s) + 6\,O_2(g) \rightarrow 6\,CO_2(g) + 6\,H_2O(l)$$

$$\Delta_cH = -2802.5\ \text{kJ}$$

F. Calculating Enthalpy Changes

- molar enthalpy, in kJ/mol, and the number of moles of a substance can be used to calculate the enthalpy change of a chemical change:

$$\boxed{\Delta_r H = \mathbf{n_r H}}$$

where: ΔrH = **enthalpy change in kJ (or J)**

n = **number of moles in mol**

$_r$H = ***molar* enthalpy in kJ/mol or J/mol**

- the number of moles can either come from the **balancing** in the chemical reaction or from the formula **$n = m/M$**

- always have a sign on ΔH or H
    - **positive** for **endothermic** (energy absorbed)
    - **negative** for **exothermic** (energy released)

Example 1

Calculate the molar enthalpy of combustion for oxygen given the following information:

$$2\ C_2H_6(g)\ +\ 7\ O_2(g)\ \rightarrow\ 4\ CO_2(g)\ +\ 6\ H_2O(g)$$

$$\Delta_cH = -2856.8\ \text{kJ}$$

$$\Delta_cH = n_cH$$

$$-2856.8\ \text{kJ} = (7\ \text{mol})_cH$$

$${}_c\mathbf{H = -\ 408.11\ kJ/mol}$$

Example 2

Find the enthalpy change when 5.50 g of pentane burns.

$_{c}H = -3244.8$ kJ/mol of pentane.

$$\Delta_{c}H = n_{c}H$$

$$= \frac{m}{M} \times {}_{c}H$$

$$= \frac{5.50\text{ g}}{72.17\text{ g/mol}} \times -3244.8\text{kJ/mol}$$

$$= -247.2828\ldots\text{kJ}$$

$$= \mathbf{-247\ kJ}$$

Example 3

When methane is burned, oxygen is consumed. Determine the mass of oxygen consumed if the change in enthalpy is –250 kJ and the molar enthalpy of reaction for oxygen is –401.3 kJ/mol.

$$\Delta_c H = \frac{m}{M} \times {}_{c}H$$

$$-250\ \text{kJ} = \frac{m}{32.00\ \text{g/mol}} \times -401.3\ \text{kJ/mol}$$

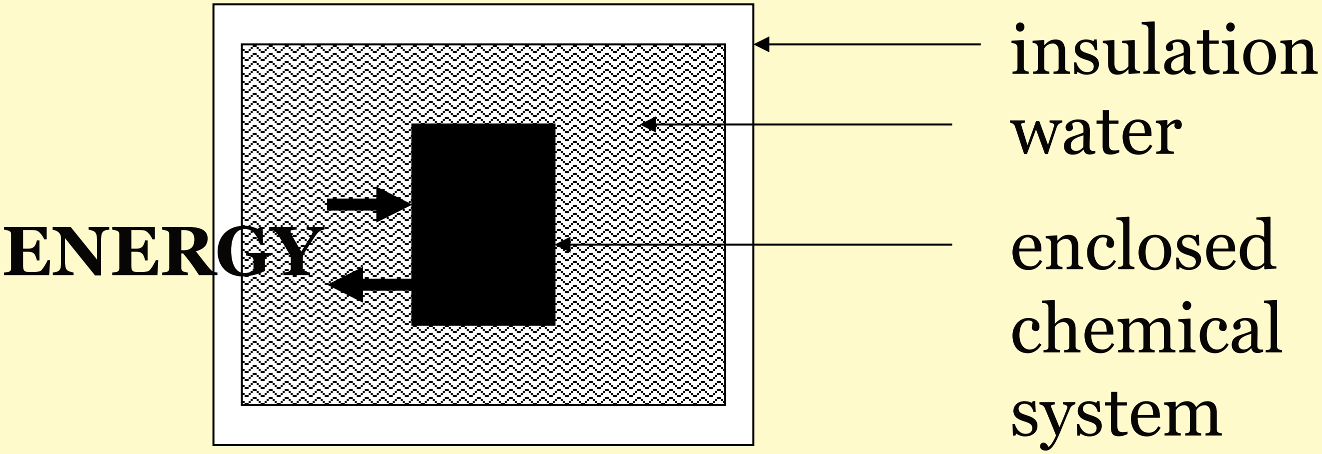
$$m = 19.935\ldots\text{g}$$

$$= \mathbf{19.9\ g}$$

G. Calorimetry

- calorimetry is a technological process of **measuring energy changes using an isolated system**
- the isolated system used to determine the heat involved in a phase change or in a chemical reaction is called a **calorimeter**

Calorimeter



Steps for Using a Simple Calorimeter

1. Measure the **initial temperature** of the water in the calorimeter.
2. Add the **reactants** to the calorimeter.
3. Allow reaction to proceed, **stirring** the solution to ensure even temperature.
4. Measure the **final temperature** of the water in the calorimeter (maximum temperature for exothermic reactions, minimum temperature for endothermic reactions)

- calorimetry is based on the First and Second Law of Thermodynamics…energy is conserved and energy is transferred from hotter objects to cooler objects until thermal equilibrium is reached

- it is assumed that **no energy** is **gained or lost** by the system except for the energy required or released by the **chemical change**

- calculations are based on the Principle of Heat Transfer:

HEAT LOST = HEAT GAINED

- remember, you must use a **sign** with your ΔH values (either enthalpy change or molar enthalpy)

endothermic = **positive** value

exothermic = **negative** value

Example 1

A chemical reaction in a bomb calorimeter causes the temperature of 500 g of water to increase in temperature from 10.0°C to 52.0°C. Calculate the heat released by this reaction. Give your answer in kJ.

$$\text{HL (rxn)} = \text{HG (water)}$$

$$= Q$$

$$= mc\Delta t$$

$$= (500\text{ g})(4.19\text{ J/g°C})(52.0\text{°C} - 10.0\text{°C})$$

$$= 87\,990\text{ J}$$

$$= -87.990\text{ kJ}$$

$$= \mathbf{-88.0\ kJ}$$

Example 2

An 8.40 g sample of $N_{2(g)}$ is reacted with pure oxygen in a bomb calorimeter containing 1.00 kg of water to produce N_2O. The temperature of the water dropped by 5.82°C. What is the molar heat of reaction of $N_{2(g)}$ in kJ/mol?

heat lost (water) = heat gained (formation)

$$Q = \Delta H$$

$$mc\Delta t = (m/M)\ H$$

$$(1000\ \text{g})(4.19\ \text{J/g°C})(5.82\text{°C}) = (8.40\ \text{g}/28.02\ \text{g/mol})\ H$$

$$24385.8\ \text{J} = (0.299\ldots\ \text{mol})\ H$$

$$H = 81344.06143\ \text{J/mol}$$

$$H = \mathbf{+81.3\ kJ/mol}$$

Example 3

A student mixes 100.0 mL of 0.500 mol/L HBr(aq) with 100.0 mL of 0.500 mol/L KOH(aq). The initial temperature of both solutions is 21.00°C and the highest temperature reached after mixing is 24.40°C. Calculate the molar enthalpy of neutralization in kJ/mol for the HBr(aq). Assume both solutions have the density and heat capacity of pure water.

heat lost (neut HBr(aq)) = heat gained (water)

$$\Delta H = Q$$

$$cv\ H = mc\Delta t$$

$$(0.1000\text{L})(0.500\ \text{mol/L})\ H = (200\text{g})(4.19\text{J/g°C})(24.40\text{°C} - 21.00\ \text{°C})$$

$$(0.0500\ \text{mol})\ H = 2849.2\ \text{J}$$

$$H = -\ 56984\ \text{J/mol}$$

$$H = \mathbf{-\ 57.0\ kJ/mol}$$

Example 4

A student built a simple calorimeter with a 25.0 g tin can and 150 mL of water. Calculate the molar enthalpy of combustion of ethanol in kJ/mol if 0.166 g of this fuel increased the temperature of the calorimeter by 7.00°C. Remember to include not only the heat gained by the water but also by the calorimeter.

heat lost (combustion) = heat gained (water + tin can)

$$\Delta H = Q$$

$$(m/M)\ H = mc\Delta t \qquad + mc\Delta t$$

$$(0.166/46.08\text{g/mol})\ H = (150\text{g})(4.19\text{J/g°C})(7.00\text{°C})$$

$$+ (25.0\text{g})(0.227\text{J/g°C})(7.00\text{°C})$$

$$(0.00360\ldots\ \text{mol})\ H = 4439.225\ \text{J}$$

$$H = -\ 1232286.057\ \text{J/mol}$$

$$H = -\ 1232.2\ldots\ \text{J/mol}$$

$$H = \mathbf{-1.23 \times 10^3\ kJ/mol}$$

H. Industrial Bomb Calorimeters

- industrial calorimeters are used in **research** to measure the heat of combustion of food, fuel, oil, crops, and explosives
- modern calorimeters have **fixed components**

  eg) volume of water used, container (bomb) material, stirrer and thermometer

- in calculating the energy of combustion, you take all components of the calorimeter into account:

$$E_{total} = mc\Delta t\,(H_2O) + mc\Delta t\,(\text{stirrer}) + mc\Delta t\,(\text{bomb}) + mc\Delta t\,(\text{thermometer})$$

- all of the “mc” parts are constant so they are replaced by **one constant C,** the **heat capacity** of the **entire system** in **kJ/°C**

- you can also be asked to calculate **kJ/g** instead of kJ/mol in calorimetry questions

- you use the formula **mH** instead of nH to give kJ/g

Example 1

A 1.50 g sample of methane is completely burned in a calorimeter with a heat capacity of 11.3 kJ/°C. The temperature increased from 20.15°C to 27.45°C. Calculate the molar enthalpy of combustion for methane.

heat lost (combustion) = heat gained (calorimeter)

$(m/M)\ H = C\Delta t$

$(1.50\text{ g}/16.05\text{ g/mol})\ H = (11.3\text{ kJ/°C})(27.45\text{°C} - 20.15\text{°C})$

$(0.0934\ \ldots\ \text{mol})\ H = 82.49\text{ kJ}$

$H = 882.6430002\text{ kJ/mol}$

$H = -$ **883 kJ/mol**

Example 2

When 3.00 g of butter is burned in a bomb calorimeter with a heat capacity of 9.22 kJ/°C the temperature changes from 19.62°C to 31.89°C. Calculate the specific enthalpy of combustion in **kJ/g**.

heat lost (combustion) = heat gained (calorimeter)

$$m\,H = C\Delta t$$

$$(3.00\text{g})\,H = (9.22\text{ kJ/°C})(31.89\text{°C} - 19.62\text{°C})$$

$$(3.00\text{ g})\,H = 113.1294\text{ kJ}$$

$$H = 37.7098\text{ kJ/g}$$

$$H = -\mathbf{37.7\ kJ/g}$$

I. Predicting Enthalpy ($\Delta_r H$) Changes
1. Using Hess's Law

- because of the law of conservation of energy, the heat of reaction is the **same** whether the reactants are converted to the products in a **single reaction** or in a **series of reactions**

- G.H. Hess (1840) suggested that if two or more **thermochemical equations** are **added** to give a final equation then the **enthalpies** can be added to give the **enthalpy for the final equation**

- sometimes the heat of reaction for a chemical change is not easily measured due to time of reaction, cost, rarity of reactants etc. so we use Hess's Law to calculate $\Delta_r H$

Steps:

1. Write the **net reaction**, if it is not given.
2. **Manipulate** the given equations so they will **add** to yield the **net equation.**
    - if you multiply or divide an equation, multiply or divide the ΔH by the **same factor**
    - if you flip an equation, **flip** the sign on ΔH
3. **Cancel** the reactants and products where possible to **simplify**
   (you should end up with your net equation!)
4. **Add** the component enthalpy changes to get the **net enthalpy change.**

Example 1

Find the heat of reaction for $C(s, di) \rightarrow C(s, gr)$ using the following reactions:

flip $C(s, gr) + O_2(g) \rightarrow CO_2(g) \quad \Delta H = -393.5\ kJ$

$C(s, di) + O_2(g) \rightarrow CO_2(g) \quad \Delta H = -395.4\ kJ$

$$C(s, di) \cancel{+ O}_2(g) \cancel{\rightarrow CO}_2(g) \qquad \Delta H = -395.4\ kJ$$

$$\cancel{CO_2(}g) \rightarrow C(s, gr) \cancel{+ O}_2(g) \qquad \Delta H = +393.5\ kJ$$

$$C(s, di) \rightarrow C(s, gr) \qquad \mathbf{\Delta H = -1.9\ kJ}$$

Example 2

Find the heat of reaction for $H_2O_2(l) \rightarrow H_2O(l) + \frac{1}{2} O_2(g)$ using the following reactions:

flip $H_2(g) + O_2(g) \rightarrow H_2O_2(l) \qquad \Delta H = -187.8\ \text{kJ}$

$H_2(g) + \frac{1}{2} O_2(g) \rightarrow H_2O(l) \qquad \Delta H = -285.8\ \text{kJ}$

$$\cancel{H_2}(g)\ \cancel{+ \tfrac{1}{2}}\ O_2(g) \rightarrow H_2O(l) \qquad \Delta H = -285.8\ \text{kJ}$$

$$H_2O_2(l) \rightarrow \cancel{H_2}(g) + \tfrac{1}{2} O_2(g) \qquad \Delta H = +187.8\ \text{kJ}$$

$$H_2O_2(l) \rightarrow H_2O(l) + \tfrac{1}{2} O_2(g) \qquad \mathbf{\Delta H = -98.0\ kJ}$$

Example 3

Find the heat of reaction for $C_{(s)} + 2 H_{2(g)} \rightarrow CH_{4(g)}$ using the following reactions:

$$\begin{array}{lll}
 & C_{(s)} + O_{2(g)} \rightarrow CO_{2(g)} & \Delta H = -393.5\text{ kJ} \\
\times 2 & H_{2(g)} + \tfrac{1}{2} O_{2(g)} \rightarrow H_2O_{(l)} & \Delta H = -285.8\text{ kJ} \\
\text{flip} & CH_{4(g)} + 2 O_{2(g)} \rightarrow CO_{2(g)} + 2 H_2O_{(l)} & \Delta H = -890.5\text{ kJ}
\end{array}$$

$$\begin{array}{ll}
C_{(s)} + \cancel{O_{2(g)}} \rightarrow \cancel{CO_{2(g)}} & \Delta H = -393.5\text{ kJ} \\
\cancel{CO_{2(g)}} + \cancel{2 H_2O_{(l)}} \rightarrow CH_{4(g)} + \cancel{2 O_{2(g)}} & \Delta H = +890.5\text{ kJ} \\
2 H_{2(g)} + \cancel{1 O_{2(g)}} \rightarrow \cancel{2 H_2O_{(l)}} & \Delta H = -571.6\text{ kJ} \\
\hline
C_{(s)} + 2 H_{2(g)} \rightarrow CH_{4(g)} & \boldsymbol{\Delta H = -74.6\text{ kJ}}
\end{array}$$

J. Using Standard Heats of Formation $\Delta_f H^\circ$

- sometimes it is not easy to measure the heat change for a reaction (too slow/expensive)

- in this case, ΔH can be determined using **heats of formation**

- *heats of formation* $({}_{f}H^{\circ})$ are the changes in E_P that occur when **compounds are formed from their elements**

- $_{f}H^\circ$ for elements cannot be directly measured therefore they are designated as **zero** …all other $_{f}H^\circ$ values are in reference to this…see pages 4-5 in data booklet

- the ΔH°_f is an indirect measure of the **stability** of a compound

✶the more **exothermic the formation** , the **more stable the compound**

(this means you have to <u>add</u> that energy to decompose it)

eg) List the following compounds in order from most stable to least stable.

3 $H_2O(l)$ $_{f}H^\circ = -285.8$ kJ/mol

5 $C_2H_4(g)$ $_{f}H^\circ = +52.4$ kJ/mol

4 $N_2O_4(g)$ $_{f}H^\circ = +11.1$ kJ/mol

2 $PCl_3(l)$ $_{f}H^\circ = -319.7$ kJ /mol

1 $Al_2O_3(s)$ $_{f}H^\circ = -1675.7$ kJ /mol

- Hess's Law formula states that the $\mathbf{\Delta_r H}$ is the difference between the standard heats of formation of the **reactants** and the **products**

$$\Delta_r H^\circ = \mathbf{\Sigma}\ \Delta_{\mathbf{f}}\mathbf{H}^\circ_{\textbf{(products)}} - \mathbf{\Sigma}\ \Delta_{\mathbf{f}}\mathbf{H}^\circ_{\textbf{(reactants)}}$$

Take the energy released during the formation of the products

And subtract the initial energy of the system (energy released when reactants were formed)

$$\Delta_r H^\circ = \mathbf{\Sigma n_f H}^\circ_{\textbf{(products)}} - \mathbf{\Sigma n_f H}^\circ_{\textbf{(reactants)}}$$

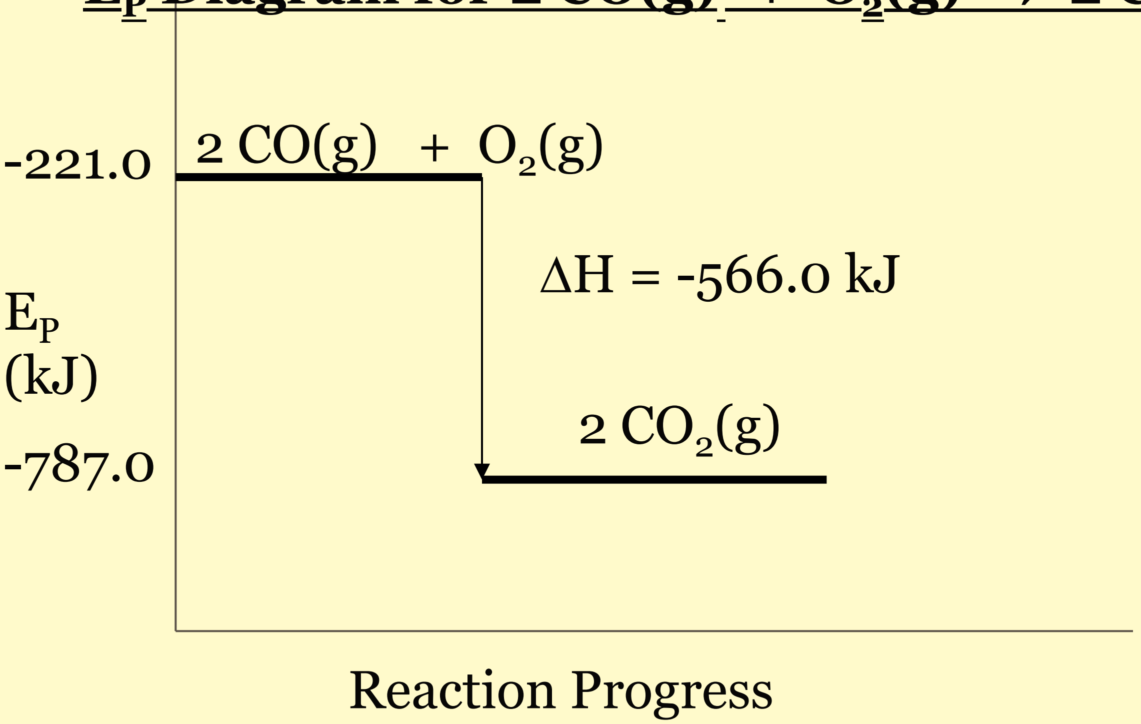
Example 1

Calculate the standard heat of combustion for $2\ CO(g) + O_2(g) \rightarrow 2\ CO_2(g)$ and draw the E_P diagram for this reaction.

$2\ CO(g)$	+	$O_2(g) \rightarrow$	$2\ CO_2(g)$
(2 mol)(-110.5 kJ/mol)	+	0 kJ	(2 mol)(-393.5 kJ/mol)
-221.0 kJ	+	0 kJ	-787.0 kJ

$$\begin{aligned} \Delta_c H^\circ &= \Sigma n_f H^\circ_{\text{(products)}} - \Sigma n_f H^\circ_{\text{(reactants)}} \\ &= -787.0\ \text{kJ} - (-221.0\ \text{kJ}) \\ &= \mathbf{-566.0\ kJ} \end{aligned}$$

E_P Diagram for $2\,CO(g) + O_2(g) \rightarrow 2\,CO_2(g)$



-221.0

$2\,CO(g) + O_2(g)$

$\Delta H = -566.0$ kJ

E_P (kJ)

$2\,CO_2(g)$

-787.0

Reaction Progress

Example 2

Find the heat of combustion of ethane and draw the EP diagram for this reaction. The products of combustion are gases.

$$2\,C_2H_6(g) \quad + \quad 7\,O_2(g) \rightarrow \quad 4\,CO_2(g) \quad + \quad 6\,H_2O(g)$$

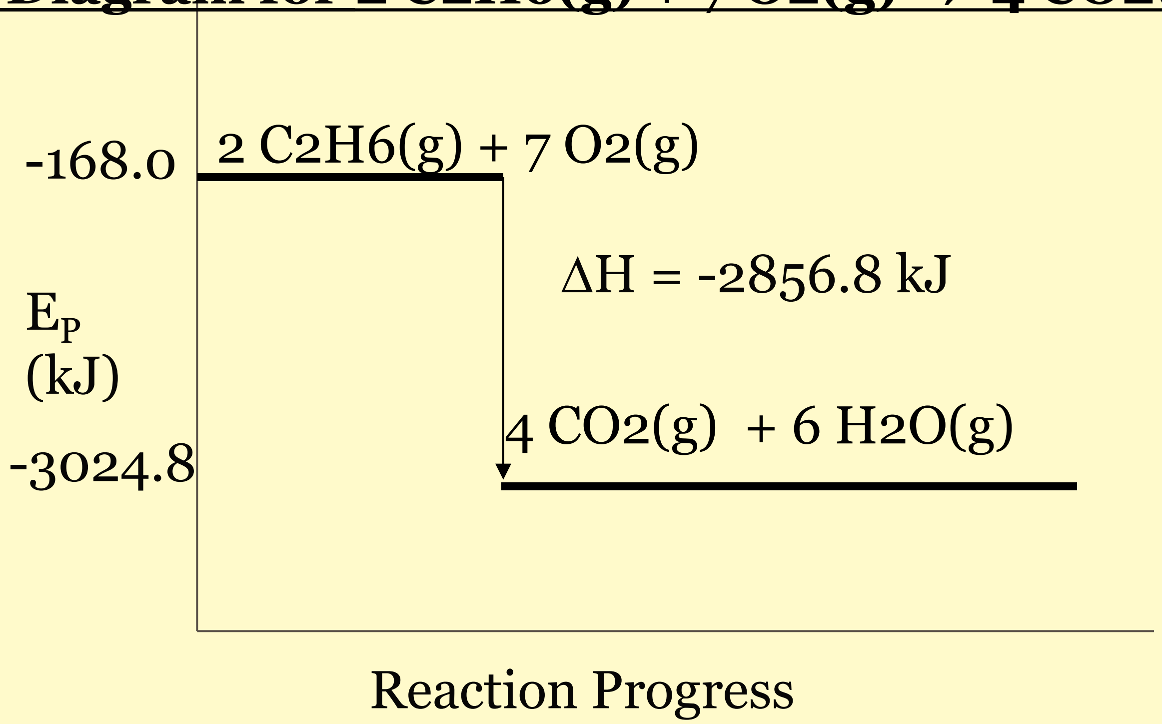
(2mol)(-84.0kJ/mol) + 0 kJ (4 mol)(-393.5 kJ/mol) +(6 mol)(-241.8 kJ/mol)

-168.0 kJ

-3024.8 kJ

$$\begin{aligned} \Delta_c H^\circ &= \Sigma n_f H^\circ_{\text{(products)}} - \Sigma n_f H^\circ_{\text{(reactants)}} \\ &= (-3024.8\ \text{kJ}) - (-168.0\ \text{kJ}) \\ &= \mathbf{-2856.8\ kJ} \end{aligned}$$

E_P Diagram for 2 $C_2H_6(g)$ + 7 $O_2(g) \rightarrow$ 4 $CO_2(g)$ + 6 $H_2O(g)$



Example 3

Calculate the molar enthalpy of combustion for ethane. The products of combustion are gases.

$$2\,C_2H_6(g) + 7\,O_2(g) \rightarrow 4\,CO_2(g) + 6\,H_2O(g)$$

$(2\text{mol})(-84.0\text{kJ/mol}) + 0\text{ kJ}$ $(4\text{ mol})(-393.5\text{ kJ/mol}) + (6\text{ mol})(-241.8\text{ kJ/mol})$

-168.0 kJ

-3024.8 kJ

$$\begin{aligned}\Delta_c H^\circ &= \Sigma n_f H^\circ_{\text{(products)}} - \Sigma n_f H^\circ_{\text{(reactants)}} \\ &= (-3024.8\text{ kJ}) - (-168.0\text{ kJ}) \\ &= -2856.8\text{ kJ}\end{aligned}$$

$$\begin{aligned}{}_cH^\circ &= \frac{\Delta_c H^\circ}{n} \\ &= \frac{-2856.8\text{ kJ}}{2\text{ mol}} \\ &= \mathbf{-1428.4\ kJ/mol}\end{aligned}$$

Example 4

Calculate the energy released when 25.0 g of methanol is burned. The products of combustion are gases.

$$2\ \mathrm{CH3OH(l)} \quad + \quad 3\ \mathrm{O_2(g)} \rightarrow 2\ \mathrm{CO_2(g)} \quad + \quad 4\ \mathrm{H_2O(g)}$$

(2mol)(-239.2kJ/mol)+ 0 kJ (2 mol)(-393.5 kJ/mol) +(4 mol)(-241.8 kJ/mol)

-478.4 kJ

-1754.2 kJ

$$\begin{aligned}\Delta\ _cH^\circ &= \Sigma n_fH^\circ{}_{\text{(products)}} - \Sigma n_fH^\circ{}_{\text{(reactants)}}\\ &= (-1754.2\ \text{kJ}) - (-478.4\ \text{kJ})\\ &= -1275.8\ \text{kJ}\end{aligned}$$

$$_{c}H^\circ = \frac{\Delta_c H^\circ}{n}$$

$$= \frac{-1275.8\ \text{kJ}}{2\ \text{mol}}$$

$$= -637.9\ \text{kJ/mol}$$

$$\Delta_c H = \frac{m}{M} \times {}_{c}H$$

$$\Delta_c H = \frac{25.0\ \text{g}}{32.05\ \text{g/mol}} \times -637.9\ \text{kJ/mol}$$

$$= \mathbf{-\ 498\ kJ}$$

Example 5

Calculate the molar heat of formation for ethylene glycol given the following information:

$$\Delta H^\circ = -1178.0\ \text{kJ}$$

$$(CH_2OH)_2(l) + 5/2\ O_2(g) \rightarrow 2\ CO_2(g) + 3\ H_2O(g)$$

(1mol)x + 0 kJ (2 mol)(-393.5 kJ/mol) +(3 mol)(-241.8 kJ/mol)

(1mol)x -1512.4 kJ

$$\begin{aligned}
\Delta H^\circ &= \Sigma n_f H^\circ_{(\text{products})} - \Sigma n_f H^\circ_{(\text{reactants})} \\
-1178.0\ \text{kJ} &= (\cancel{-1512.4}\ \text{kJ}) - (1\ \text{mol})x \\
+\ 1512.4 &= \cancel{+1512.4} \\
\frac{+334.4\ \text{kJ}}{(-1\ \text{mol})} &= \frac{-\ (1\ \cancel{\text{mol}})x}{(\cancel{-1}\ \text{mol})} \\
x &= \mathbf{-334.4\ kJ/mol}
\end{aligned}$$

K. Energy and Efficiency

- most of Canada's energy (electricity) comes from **chemical** processes such as the combustion of **fossil fuels**

- electricity is also generated through **nuclear** processes

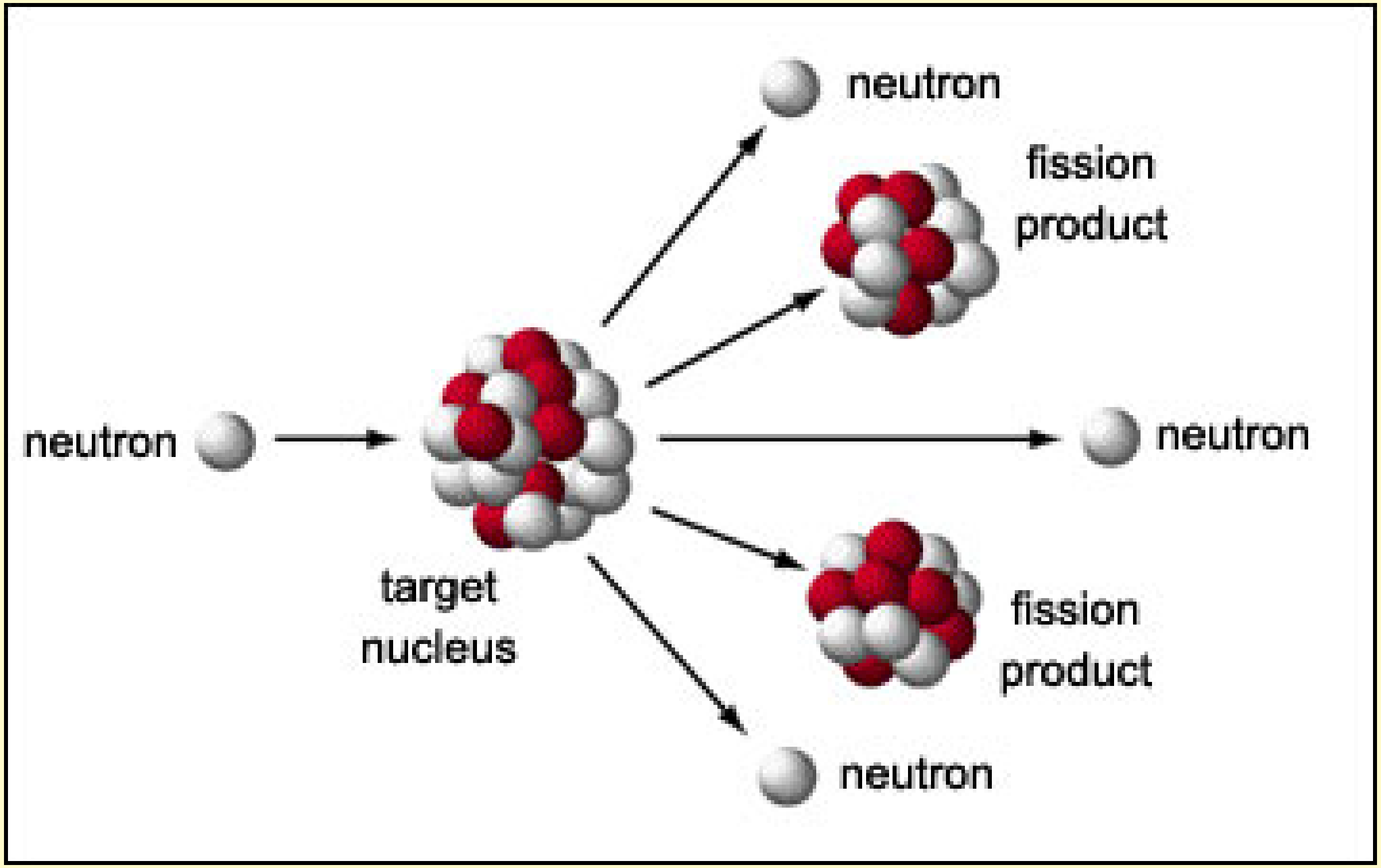
- both methods involve changing **water into steam** (a **phase** change) which turns turbines to generate electrical energy

- how does the energy from physical, chemical and nuclear processes compare:

  - **physical** changes involve the breaking and forming of **intermolecular** forces (**1 – 100** kJ/mol)

- **chemical** changes involve the breaking and forming of **chemical bonds** (**100 – 10000** kJ/mol)

- **nuclear** changes involve changes within the **nuclei of atoms** (**millions to billions** kJ/mol)



- **efficiency** is the ratio of **useful energy** produced (energy **output**) to **energy used** in its production (energy **input**)

$$\boxed{\%\ \text{Efficiency} = \frac{\text{Energy output}}{\text{Energy input}} \times 100}$$

- we have developed many technologies that help us to solve practical problems
- it is important to be as **efficient** as possible with appliances and vehicles

- saving energy **saves you money** and it helps to **save the environment** (greenhouse effect and acid rain)

- in any process, the **more energy conversions** that take place, the **less efficient** the process because of **heat loss** in transfer

- gas furnace (natural gas) is about **90%** efficient since it is used to directly supply heat

- natural gas power plant is only about **37%** efficient because there are several energy conversions that take place before electricity is generated (water to steam to kinetic energy to mechanical energy to electrical energy)

L. Fuelling Society

- we must assess the **risks and benefits** of relying on any fuel source
- when selecting an energy source, efficiency is not the only consideration
- **environmental impact** must also be considered

Advantages vs. Disadvantages of Fossil Fuels

Advantages

- relatively low cost
- readily available (market)
- plant set-up, vehicle design, expertise affordable
- used all over the world
- deposits are large

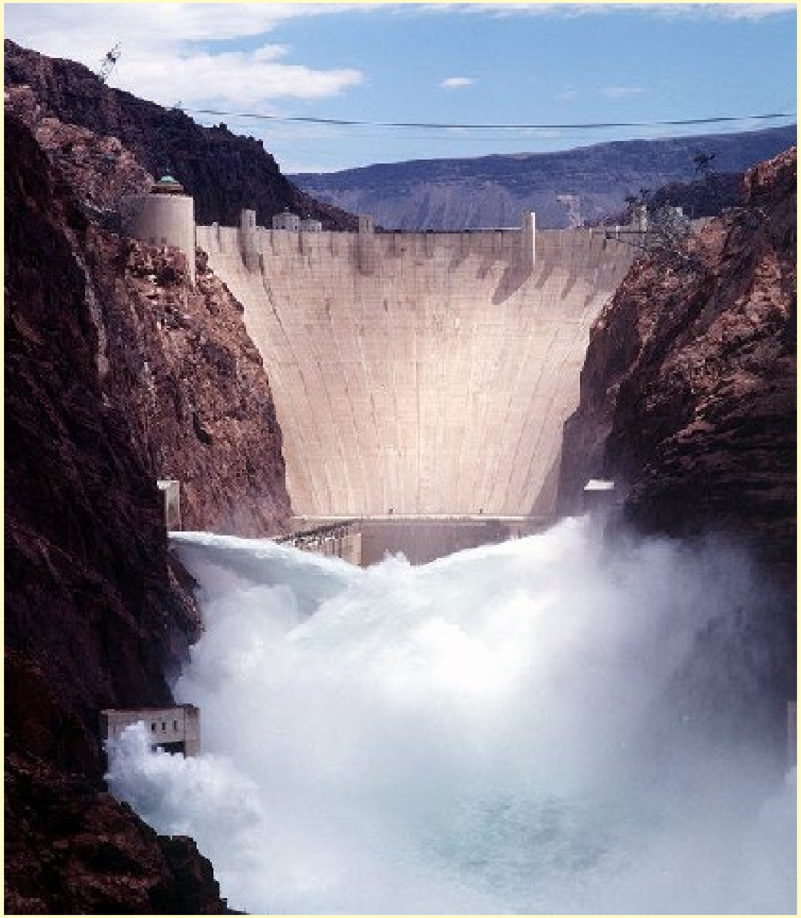
Disadvantages

- release of gases that contribute to the greenhouse effect and acid rain when burned
- mining is detrimental to the environment
- non-renewable

- **nuclear** processes **do not** produce **greenhouse gases** but they do produce **radioactive waste** which lasts for thousands of years

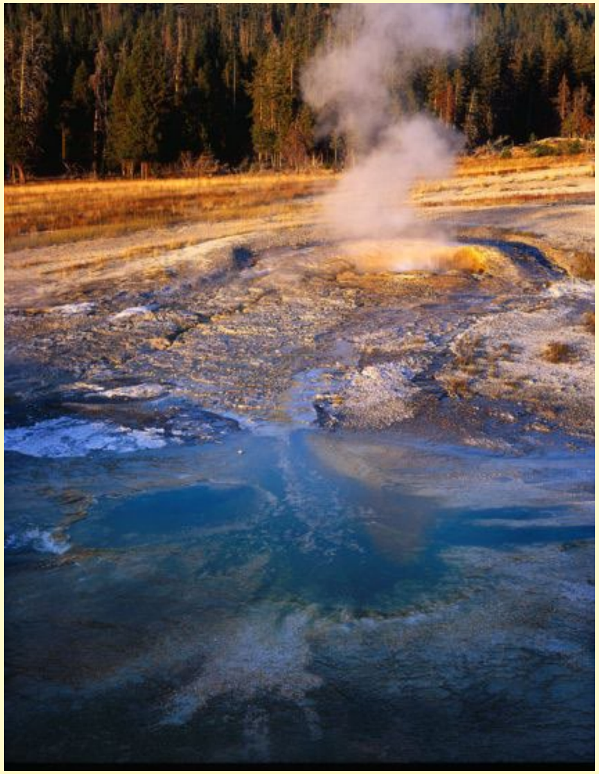
- **wind** turbines use a **renewable** energy source (sun indirectly) but are not free of problems…they are **noisy and dangerous to birds**

- **hydroelectric** power is also **renewable** but damming rivers **affects ecosystems** on both sides of the dams



- the amount of **$CO_2(g)$** released by a fuel determines how **“clean”** it is

- fuels that use renewable energy sources (**solar, wind, geothermal** etc.) and nuclear power are considered the **“cleanest”**



- **methane** is the **“cleanest”** fossil fuel and **coal** is the **least clean**

- regardless of which source of energy we use, we must think about the impact that our fuels have on the environment

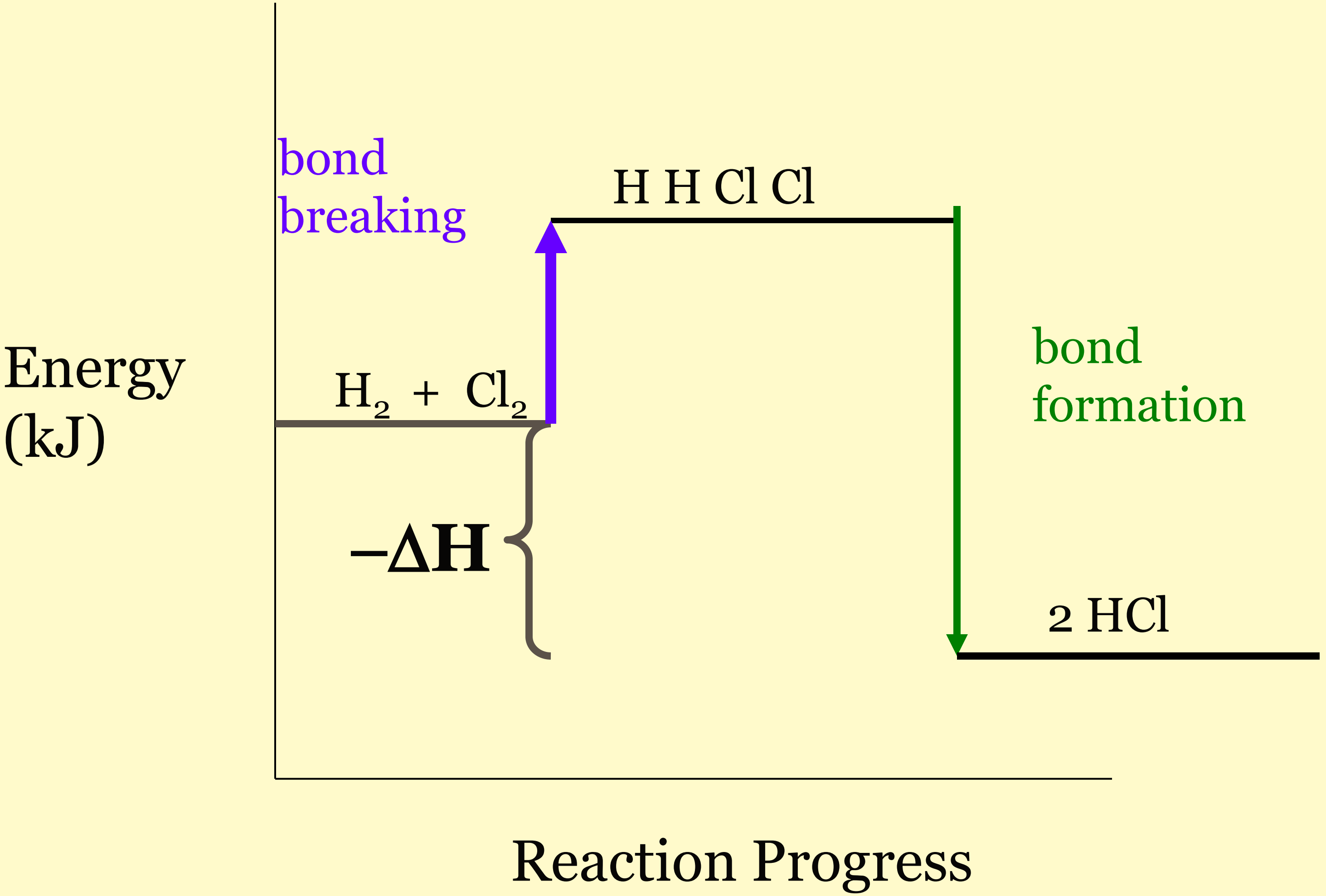
M. Bond Energy and Activation Energy

- bond energy is the energy **required to break a chemical bond** or the energy **released when a bond is formed**

- the **change in enthalpy** of a reaction represents the **net effect** from **breaking** the bonds in the reactant(s) and **forming** the bonds of the product(s)

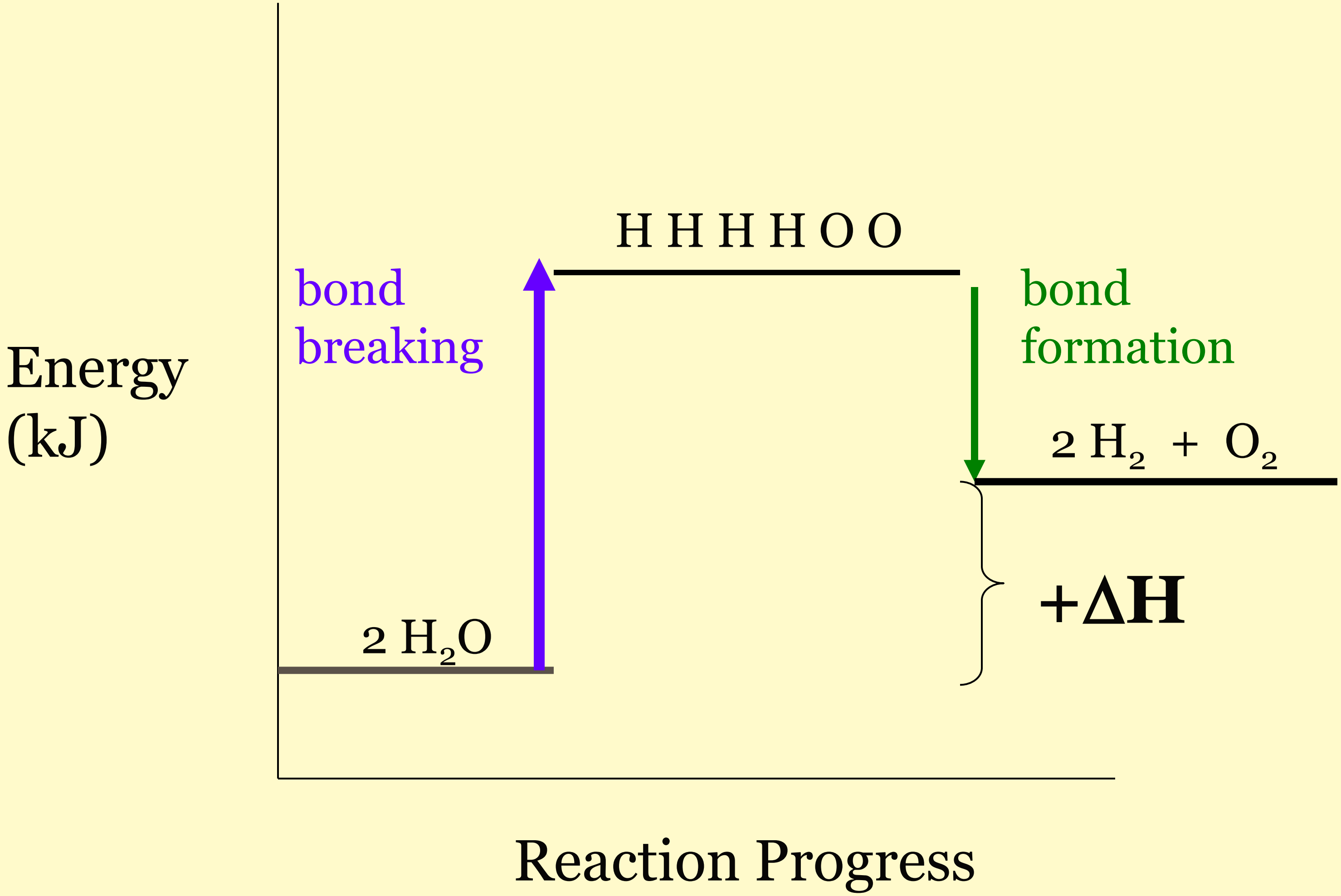
- in **exothermic** reactions, bond breaking absorbs **less** energy than the bond formation gives off, resulting in a **$-\Delta H$**

Exothermic $H_2\,(g) + Cl_2\,(g) \rightarrow 2\,HCl\,(g) + \text{energy}$



- in **endothermic** reactions, bond breaking absorbs **more** energy than the bond formation gives off, resulting in a **+ΔH**

Endothermic $2\ H_2O(l)\ +\ \text{energy} \rightarrow 2\ H_2\ (g) + O_2\ (g)$



- the energy barrier that must be overcome for a chemical reaction to occur is called the **activation energy**

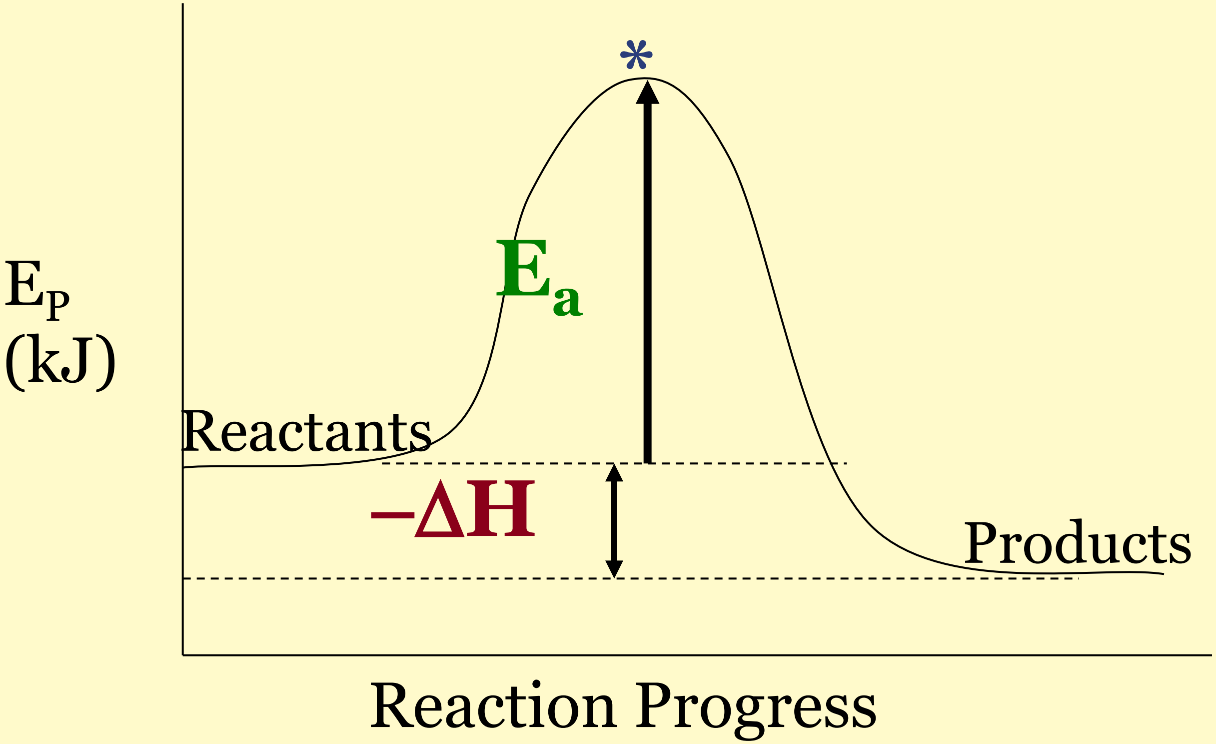
- the atoms in the **reactants** have to be **“pulled apart”** in order for them to bond in a different configuration and become the products

- the activation energy is always **higher** than the energy contained in the reactants and the products, however the amount of activation energy necessary is dependent on the reaction

- the **top** of the activation energy barrier on a potential energy diagram represents the **changeover point** of the reaction
- in both endothermic and exothermic reactions, the molecules of the reactants are moving with a certain amount of **kinetic energy**
- when the reactants **collide** with each other, the kinetic energy is transformed into **potential energy**

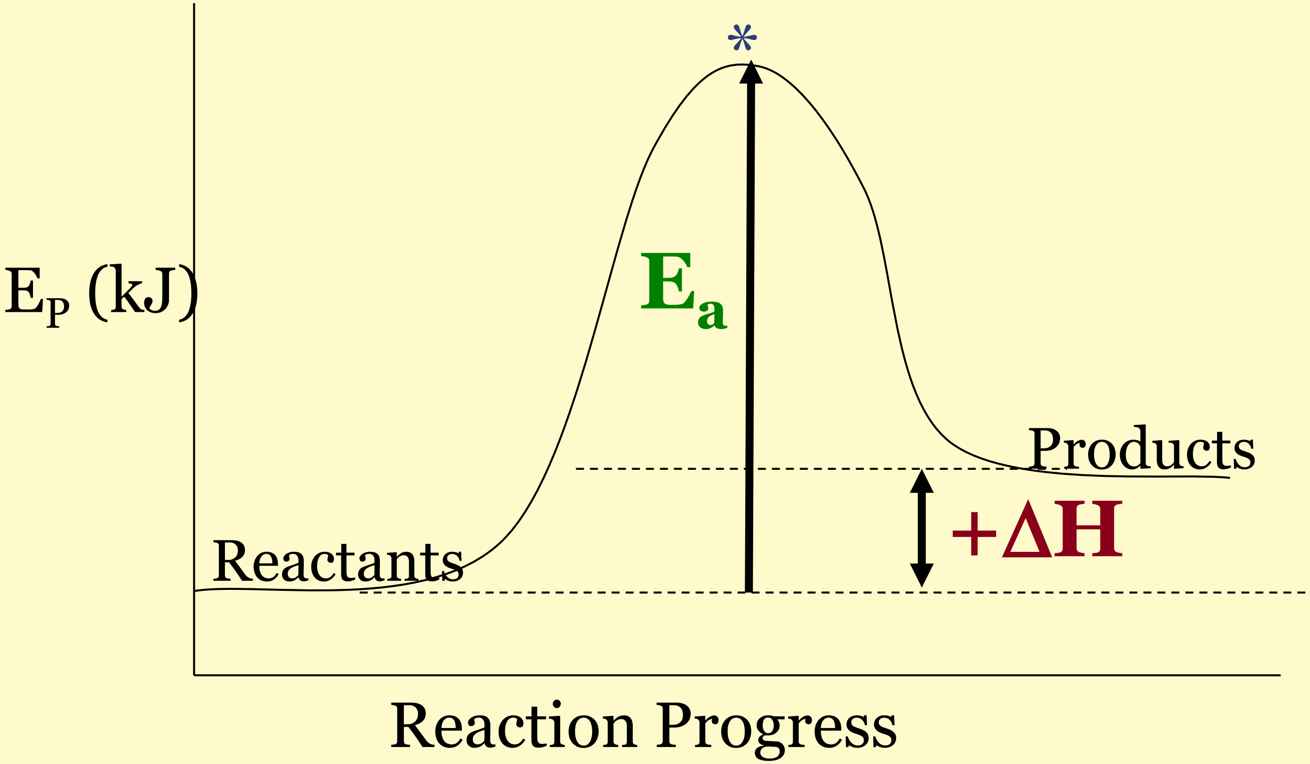
- this potential energy is then stored in bonds of the chemical species that exists at the top which is called the **activated complex**
- this is a transitional species that is neither a reactant nor a product which has **partial bonds** and is **highly unstable**
- when the partial bonds of the activated complex re-form as chemical bonds in the products, the stored potential energy is converted back into **kinetic energy** as the product molecules **move apart**

Potential Energy Diagram: Exothermic



* **activated complex**

Potential Energy Diagram: Endothermic

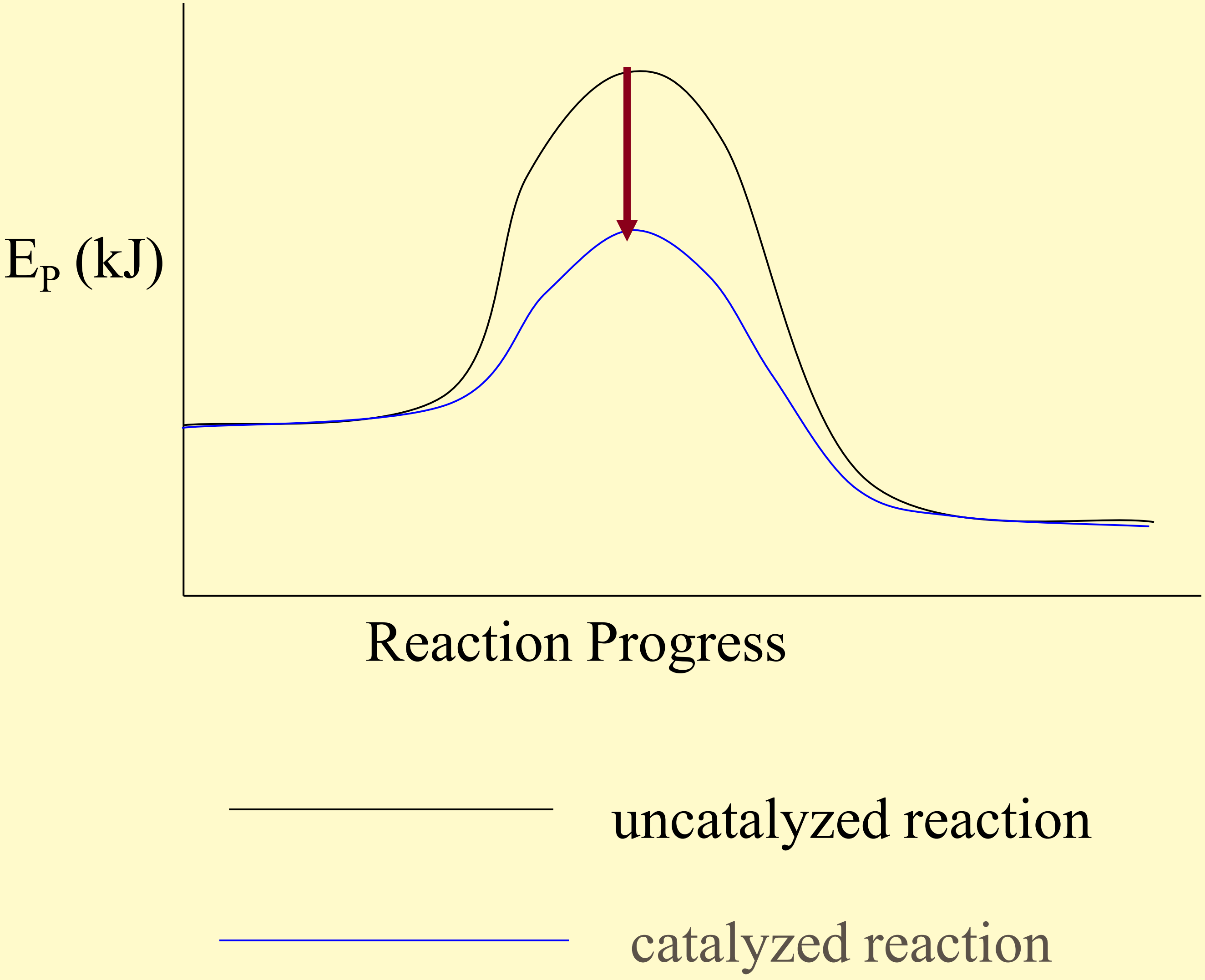


* **activated complex**

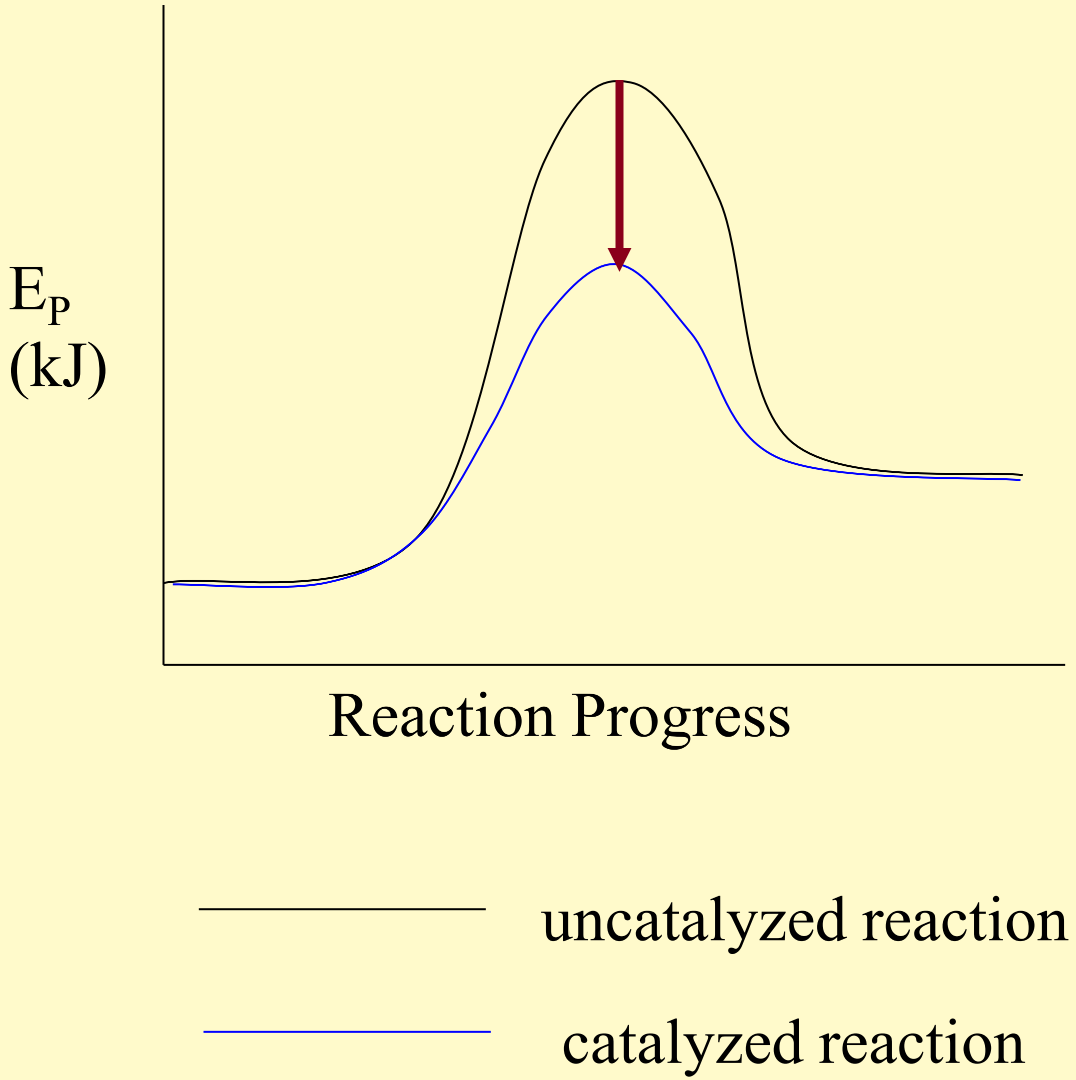
N. Catalysts

- ✶ a catalyst is a substance that **increases the rate** of a chemical reaction **without being consumed** by the reaction
- ✶ catalysts provide **alternate pathways** for chemical reactions
- ✶ they **lower** the **activation energy** required for a reaction to take place which results in the production of a **greater yield** of products in a given length of time (even at a lower temperature)
- ✶ catalyzed reactions can be shown on E_P diagrams:

Potential Energy Diagram: Exothermic



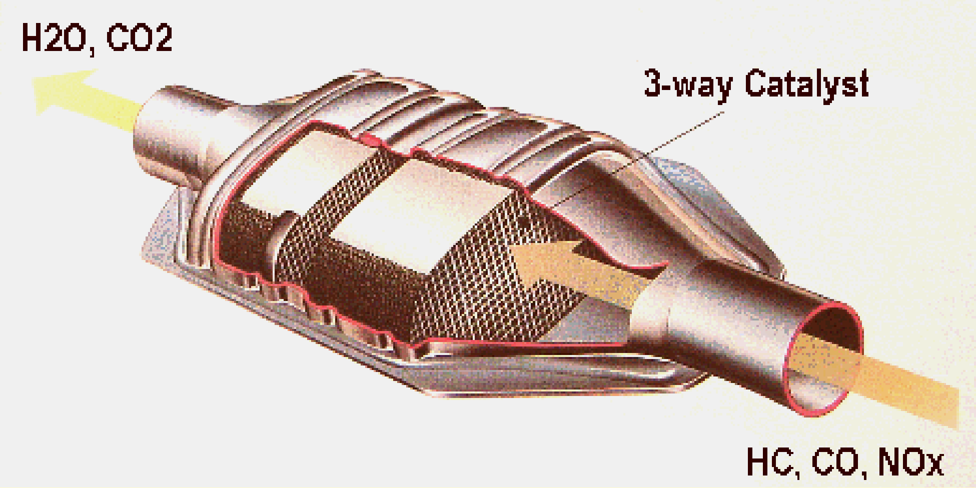
Potential Energy Diagram: Endothermic



O. Catalysts in Industry

- catalysts are often used in industry to speed up the reactions and obtain a reasonable reaction rate under reasonable conditions

- in cars, we have **catalytic converters** that use Pt(s), Pd(s) and Rh(s) to speed up the combustion of exhaust gases so that more of the products are **harmless** ($\mathbf{N_2}$ instead of $\mathbf{NO_x}$, $\mathbf{CO_2}$ instead of **CO**)



- the oil and gas industry uses catalysts (Pt(s), HF(aq), H_2SO_4(aq) etc) in the **cracking and reforming** of **crude oil** and **bitumen** to make more marketable fuels like gasoline

P. Enzymes

- compounds that act as catalysts in living systems are called **enzymes**
- called **biological** catalysts

  eg) amylase, peptidase, lactase

- chemical reactions in the body occur at very **low** temperature (37°C) and without catalysts many would be too **slow**