Bond Enthalpy and Activation Energy
Energy of a Chemical Reaction

- $\Delta H = \sum \Delta H_{(bonds \ broken)} - \sum \Delta H_{(bonds \ formed)}$

- Add up all the energies of the broken bonds
- Add up all the energies of the bonds that are reformed
- Subtract the difference and that is the net energy of the reaction.
# Bond Enthalpies

## Average Bond Enthalpies (kJ/mol)

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## Multiple Bonds

| C—N          | 614  |      |      |      |      |      |      |       |       |      |      |      |       |       |      |       |
| C—O          |      |      |      |      |      |      |      |       |       |      |      |      |       |       |      |       |
| Si—Si        |      |      |      |      |      |      |      |       |       |      |      |      |       |       |      |       |
| Si—C         |      |      |      |      |      |      |      |       |       |      |      |      |       |       |      |       |
| Si—O         |      |      |      |      |      |      |      |       |       |      |      |      |       |       |      |       |

### General Notes
- **Bond Enthalpies** are the energy changes associated with the formation of chemical bonds.
- The table lists the average bond enthalpies for various bonds, measured in kJ/mol.
Exothermic vs. Endothermic

• If the final $\Delta H$ is negative, then it is an exothermic reaction.

• Energy released is $-\Delta H$ because it is leaving the system. There is less energy than before.

• If the final $\Delta H$ is positive, then it is an endothermic reaction.

• Energy released is $+\Delta H$ because it is joining the system. There is more energy than before.
Example One

• $2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$

$$
\begin{align*}
\text{H-H} & = 436 \text{ KJ/mol} \\
\text{O=O} & = 498 \text{ KJ/mol} \\
\text{H-O} & = 463 \text{ KJ/mol}
\end{align*}
$$

$$
\Delta H = \sum \Delta H_{(bonds \ broken)} - \sum \Delta H_{(bonds \ formed)}
$$

$$
\begin{align*}
\Delta H &= [2(436) + 498] - [4(463)] \\
&= 1367 - 1852 = -482 \text{ KJ/mol}
\end{align*}
$$
Example One

• $2H_2 + O_2 \rightarrow 2H_2O$

$\Delta H = [2(436) + 498] - [4(463)] = 1367 - 1852 = \text{-482 KJ/mol}$

This is an exothermic reaction!
Getting Chemical Reactions Going

- **Activation energy** is the term for the energy needed to break the bonds so new bonds can form.
Activation Energy

- The net energy difference is the $\Delta H$. But, first you must add activation energy to initially break the chemical bonds.
Catalysts

• Catalysts simply lower the activation energy needed to do the chemical reaction going.
Catalyst

- Catalysts provide a surface for chemical reactions to occur without themselves being used up in the reaction.
Getting Chemical Reactions Going

- **Energy** is usually needed to break the bonds and get the reaction going.
- This can be a spark, flame, heat, or even a feather.
Getting Chemical Reactions Going

- **Activation energy** is the energy needed to break the bonds so new bonds can form.
Example Question

What is the enthalpy value of the equation below:

\[ \text{C}_2\text{H}_2 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]
Example Question

What is the enthalpy value of the equation below:

$2\text{C}_2\text{H}_2 + 5\text{O}_2 \rightarrow 4\text{CO}_2 + 2\text{H}_2\text{O}$

\[
\begin{align*}
2 \text{C≡C} & \rightarrow +839*2 \\
4 \text{C-H} & \rightarrow +413*4 \\
5 \text{O=O} & \rightarrow +498*3
\end{align*}
\]

\begin{align*}
\text{Total} & = +5820 \text{ kJ} \\
\end{align*}

\[
\begin{align*}
8 \text{C=O} & \rightarrow -804*8 \\
4 \text{H-O} & \rightarrow -463*4
\end{align*}
\]

\begin{align*}
\text{Total} & = -8284 \text{ kJ} \\
\Delta \text{H} & = -2464 \text{ kJ}
\end{align*}

But, despite the /mol it is for the entire equation or -1232 kJ/mol of C$_2$H$_2$. 
Example Question

What is the enthalpy value of the equation below:

What about 10 g of acetylene?

\[ 2\text{C}_2\text{H}_2 + 5\text{O}_2 \rightarrow 4\text{CO}_2 + 2\text{H}_2\text{O} \]

\[ \begin{align*}
2 \text{C≡C} & \rightarrow +839\times 2 \\
4 \text{C-H} & \rightarrow +413\times 4 \\
5 \text{O=O} & \rightarrow +498\times 3 \\
\hline
+5820 \text{ kJ} & \quad -8284 \text{ kJ} \\
\hline
\end{align*} \]

\[ \Delta H = -2464 \text{ kJ} \]

But, despite the /mol it is for the entire equation or -1232 kJ/mol of \text{C}_2\text{H}_2.
Bond Enthalpy Example #2

• What is the $\Delta H$ for the decomposition of NI$_3$?

• NI$_3 \rightarrow$ N$_2$ + I$_2$

• N-I bond is 169 kJ/mol
Entrance Question #1

What is the enthalpy change for this reaction and is it endothermic or exothermic?

\[ \text{H}_2(g) + \text{I}_2(g) \rightarrow 2\text{HI}(g) \]
Entrance Question #1

What is the enthalpy change for this reaction and is it endothermic or exothermic?

\[ H_2(g) + I_2(g) \rightarrow 2HI(g) \]

H-H = +436 kJ/mol
I-I = +151 kJ/mol

+587 kJ/mol to break bonds
Entrance Question #1

What is the enthalpy change for this reaction and is it endothermic or exothermic?

\[ H_2(g) + I_2(g) \rightarrow 2HI(g) \]

+587 kJ/mol to break bonds

\[ 2 \text{ H-I} = -299 \times 2 = -598 \text{ kJ/mol} \]

\[ \Delta H = -12 \text{ kJ/mol} \]
Entrance Question #1

Which “mole” does kJ/mol refer to?

• kJ/mol refers to the balanced equation as a whole.
• If you are focused on one particular substance, you need to divide it by that coefficient.

What is the enthalpy change for this reaction and is it endothermic or exothermic?

\[ H_2(g) + I_2(g) \rightarrow 2HI(g) \]

• +587 kJ/mol to break bonds
• \[ 2 \text{ H-I} = -299 \times 2 = -598 \text{ kJ/mol} \]
• \[ \Delta H = -12 \text{ kJ/mol} \]
Entrance Question #1
What is the ΔH per mole of HI produced?

• Since -12 kJ/mol refers to 2 moles of HI, divide by 2 to get -6 kJ/mol of HI molecules.

What is the enthalpy change for this reaction and is it endothermic or exothermic?

\[ H_2(g) + I_2(g) \rightarrow 2HI(g) \]

• +587 kJ/mol to break bonds
• \[ 2 \text{ H-I} = -299 \times 2 = -598 \]
  
  kJ/mol
• \[ \Delta H = -12 \text{ kJ/mol} \]
### Endothermic and Exothermic Reactions

<table>
<thead>
<tr>
<th></th>
<th>Exothermic Reactions</th>
<th>Endothermic Reactions</th>
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<tbody>
<tr>
<td><strong>Energy</strong></td>
<td>Energy is Released to the Surroundings</td>
<td>Energy is Absorbed from the Surroundings</td>
</tr>
<tr>
<td><strong>Signs</strong></td>
<td>Gets Hot Flame Light produced</td>
<td>Gets Cold</td>
</tr>
<tr>
<td><strong>Examples</strong></td>
<td>Combustion of Methane</td>
<td>Cold Pack Photosynthesis</td>
</tr>
</tbody>
</table>

**Energy is Released to the Surroundings**
- Gets Hot
- Flame
- Light produced

**Energy is Absorbed from the Surroundings**
- Gets Cold
- Dark color
## Factors That Influence Reaction Rates

<table>
<thead>
<tr>
<th>Catalyst</th>
<th>Increases the Reaction Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Concentration of Reactants</strong></td>
<td>Increase in Concentration increases the reaction rate because of an increase in particle collisions.</td>
</tr>
<tr>
<td><strong>Surface Area</strong></td>
<td>More surface area increases the reaction rate. (Smaller particles give a greater overall surface area when all the particles surfaces are added together.)</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>Increase in Temperature increases the reaction rate because of an increase in particle collisions.</td>
</tr>
<tr>
<td><strong>Stirring</strong></td>
<td>Increases the Reaction Rate by increasing the number of collisions.</td>
</tr>
</tbody>
</table>
Concentration

• Higher concentrations mean more collisions of molecules and a faster reaction rate.
Surface Area

• Powdered forms are much more reactive than solid because there is a larger surface area for the reaction to occur.
Temperature

• We cook food to make the chemical reactions occur more quickly that denature proteins and make it more edible/digestible.
Stirring

• Stirring moves the particles around and speeds up the rate of collisions.
## Factors That Influence Reaction Rates

<table>
<thead>
<tr>
<th>Factor</th>
<th>Affect on Reaction Rate</th>
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<tbody>
<tr>
<td>Catalyst</td>
<td>![Catalyst Image]</td>
</tr>
<tr>
<td>Concentration of Reactants</td>
<td>![Concentration Image]</td>
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<tr>
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<td>![Temperature Image]</td>
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<tr>
<td>Stirring</td>
<td>![Stirring Image]</td>
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</table>
Many Chemical Reactions Can Be Reversed

- If energy is added to a system, chemical reactions can be reversed. These would by definition be endothermic reactions.

- In Entropy, we’ll discuss spontaneity and the likelihood of reversal.
EXAMPLE

The complete combustion of propane can be represented by the following equation: \( \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} \)

It’s helpful to draw the molecules, so you can see which bonds are present to be broken and reformed.

The Bond Enthalpies Are:

\[ \text{C-H} = 413 \quad \text{C-C} = 347 \quad \text{O=O} = 498 \quad \text{C=O} = 805 \quad \text{H-O} = 464 \]
Example

The complete combustion of propane can be represented by the following equation: \( C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O \)

The Bond Enthalpies Are:

<table>
<thead>
<tr>
<th>Bond</th>
<th>Enthalpy (kJ/mol)</th>
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<tbody>
<tr>
<td>C-H</td>
<td>413</td>
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<td>C-C</td>
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<tr>
<td>C=O</td>
<td>805</td>
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<tr>
<td>H-O</td>
<td>464</td>
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</table>

\[
\Delta H = \sum \Delta H_{\text{bonds broken}} - \sum \Delta H_{\text{bonds formed}}
\]

\[
[8(413) + 2(347) + 5(498)] - [6(805) + 8(464)] = -2054 \text{ KJ/mol}
\]

Burning Propane Is Highly Exothermic
Entrance Question: Bond Enthalpy

• How much energy can be produced by burning 5 grams of kerosene (C_{14}H_{30})?

• C_{14}H_{30} + O_2 \rightarrow CO_2 + H_2O

• 2C_{14}H_{30} + 43O_2 \rightarrow 28CO_2 + 30H_2O
Entrance Question: Bond Enthalpy

• How much energy can be produced by burning 5 grams of kerosene (C_{14}H_{30})?

\[2C_{14}H_{30} + 43O_2 \rightarrow 28CO_2 + 30H_2O?\]

• \(26 \text{ C-C}\)

• \(56 \text{ C}=\text{O}\)

• \(60 \text{ C-H}\)

• \(60 \text{ O-H}\)

• \(43 \text{ O}=\text{O}\)

\[\begin{align*}
\text{Energy released} &= [(26 \times 348) + (60 \times 413) + (43 \times 495)] - [(56 \times 804) + (60 \times 463)] =
\end{align*}\]

\[\begin{align*}
55113 - 72804 &= -17691 \text{ kJ}
\end{align*}\]

• -8845.5 kJ/mol of kerosene

• 5 g / 198 g/mol = 0.02525 mol

• 0.02525 mol * -8845.5 kJ/mol = -223.35 kJ