Lecture 17
Chapter 6

• Announcements
• Bond Energies
• Chemical reactions
• Calorimetry
• Enthalpy
• World energy consumption
Bond Energies

- Bond energy (BE) – energy required to break a bond, always positive
- Usually expressed in kJ/mol

\[ \text{H}_2 (g) \rightarrow \text{H} (g) + \text{H} (g) \quad \Delta E_{\text{bond breaking}} = \text{BE} = +435 \text{ kJ/mol} \]

(must put energy into system to break bond = positive)

And the reverse process:

\[ \text{H} (g) + \text{H} (g) \rightarrow \text{H}_2 (g) \quad \Delta E_{\text{bond making}} = - \text{BE} = -435 \text{ kJ/mol} \]

(get energy out of system when making bond = negative)
### Table 6 – 2: Average Bond Energies

<table>
<thead>
<tr>
<th>Diatomic Molecules (Dissociation Energy of Gaseous Molecules)</th>
<th></th>
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<tbody>
<tr>
<td>H—H</td>
<td>435</td>
<td></td>
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<tr>
<td>F—F</td>
<td>155</td>
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</tr>
<tr>
<td>O＝O</td>
<td>495</td>
<td></td>
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<tr>
<td>H—F</td>
<td>565</td>
<td></td>
</tr>
<tr>
<td>Cl—Cl</td>
<td>240</td>
<td></td>
</tr>
<tr>
<td>N＝O</td>
<td>605</td>
<td></td>
</tr>
<tr>
<td>H—Cl</td>
<td>430</td>
<td></td>
</tr>
<tr>
<td>Br—Br</td>
<td>190</td>
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</tr>
<tr>
<td>N＝N</td>
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<td></td>
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<tr>
<td>H—Br</td>
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<td></td>
</tr>
<tr>
<td>I—I</td>
<td>150</td>
<td></td>
</tr>
<tr>
<td>C＝O</td>
<td>1070</td>
<td></td>
</tr>
<tr>
<td>H—I</td>
<td>295</td>
<td></td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Single Covalent Bonds (Average Values)</th>
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<tbody>
<tr>
<td>H—C</td>
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</tr>
<tr>
<td>C—C</td>
<td>345</td>
<td></td>
</tr>
<tr>
<td>Si—Si</td>
<td>225</td>
<td></td>
</tr>
<tr>
<td>N＝N</td>
<td>160</td>
<td></td>
</tr>
<tr>
<td>O＝O</td>
<td>145</td>
<td></td>
</tr>
<tr>
<td>H—N</td>
<td>390</td>
<td></td>
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<tr>
<td>C—N</td>
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<td></td>
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<tr>
<td>Si—F</td>
<td>565</td>
<td></td>
</tr>
<tr>
<td>N＝O</td>
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<tr>
<td>O＝Si</td>
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<tr>
<td>H—O</td>
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<tr>
<td>C—O</td>
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<td>Si—Cl</td>
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<td>O＝P</td>
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<td>C—Si</td>
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<td>Si—Br</td>
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<td>C—P</td>
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<td>Si—N</td>
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<td>P＝P</td>
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<td>O＝Cl</td>
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<tr>
<td>H—S</td>
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<td>C—S</td>
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<td>Sn—Sn</td>
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<td>O＝Br</td>
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<td>H—Te</td>
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<tr>
<td>C—F</td>
<td>485</td>
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<tr>
<td>Sn—Cl</td>
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<tr>
<td>P＝Cl</td>
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<tr>
<td>S＝O</td>
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<td>C—Br</td>
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<tr>
<td>P＝I</td>
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<tr>
<td>S＝S</td>
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</tr>
<tr>
<td>C—I</td>
<td>215</td>
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</table>

<table>
<thead>
<tr>
<th>Multiple Covalent Bonds (Average Values)</th>
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<tbody>
<tr>
<td>C＝C</td>
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<tr>
<td>N＝N</td>
<td>420</td>
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<tr>
<td>C＝O</td>
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<td></td>
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<tr>
<td>C＝N</td>
<td>615</td>
<td></td>
</tr>
<tr>
<td>N＝O</td>
<td>605</td>
<td></td>
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<tr>
<td>C＝N</td>
<td>890</td>
<td></td>
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<tr>
<td>C＝O O＝P</td>
<td>750</td>
<td>545</td>
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<tr>
<td>C＝S</td>
<td>575</td>
<td>515</td>
</tr>
<tr>
<td>O＝S</td>
<td>515</td>
<td></td>
</tr>
</tbody>
</table>

* All values are in kilojoules per mole (kJ/mol) and are rounded to the nearest 5 kJ/mol.

† C＝O bond energy in CO₂
Reaction Energy

- Bond energies can be used to estimate the energy change that occurs in a chemical reaction

\[ \Delta E_{rxn} = \sum BE_{(bonds\ broken)} - \sum BE_{(bonds\ formed)} \]

- Strategy = count up all types of bonds in reactants (broken) and all types of bonds in products (made), then plug into formula.
How much energy is released when 1 mole of methanol is burned?

<table>
<thead>
<tr>
<th>25%</th>
<th>1.</th>
<th>1160 kJ</th>
<th>2.</th>
<th>2315 kJ</th>
<th>3.</th>
<th>4565 kJ</th>
<th>4.</th>
<th>6880 kJ</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
</tbody>
</table>
Methanol Combustion

\[ 2\text{CH}_3\text{OH} + 3\text{O}_2 \rightarrow 2\text{CO}_2 + 4\text{H}_2\text{O} \]

List bonds broken and made

<table>
<thead>
<tr>
<th>Broken</th>
<th>Made</th>
</tr>
</thead>
<tbody>
<tr>
<td>6 C-H (415 kJ each)</td>
<td>4 C=O (800 kJ each)</td>
</tr>
<tr>
<td>2 C-O (360 kJ each)</td>
<td>8 O-H (460 kJ each)</td>
</tr>
<tr>
<td>2 O-H (460 kJ each)</td>
<td></td>
</tr>
<tr>
<td>3 O-O (145 kJ each)</td>
<td></td>
</tr>
</tbody>
</table>

Total 4565 kJ 6880 kJ
(per 2 moles of methanol)
Measuring Energy Changes: Calorimetry

- **Calorimeter**: a device used to measure heat flows that accompany chemical processes.
- A Styrofoam cup is a simple calorimeter (in lab later)
- **Exothermic**: if chemicals in the calorimeter release heat.
- **Endothermic**: if chemicals in the calorimeter absorb heat.

\[ q_{\text{chemicals}} = - q_{\text{calorimeter}} \]

\[ q_{\text{calorimeter}} = C_{\text{cal}} \Delta T \]

So, measure \( \Delta T \) – this allows \( q_{\text{calorimeter}} \) to be calculated, and one can deduce \( q_{\text{chemicals}} \).
Most reactions occur at constant pressure

- It would be nice to have an easy way to measure the heat change of a chemical reaction.
- But, \( \Delta E = q + w \) so heat is not energy
- So, let’s define a new thermodynamic function – enthalpy

- Definition of enthalpy \( H = E + PV \)
- Turns out that if \( p \) is constant, then \( H = q \)

- Text derives this for you (pp. 237-238)

- Enthalpy is a state function
Enthalpy

• In practice, enthalpy can be calculated by

\[ \Delta H_{\text{reaction}} = \Delta E_{\text{reaction}} + RT\Delta n_{\text{gases}} \]

(for constant \( p \) and constant \( T \))

\[ \Delta n_{\text{gases}} = n_{\text{gas products}} - n_{\text{gas reactants}} \]

So, if no gases are produced or consumed, and \( p \) and \( T \) are constant, then

\[ \Delta H_{\text{reaction}} = \Delta E_{\text{reaction}} \]
Enthalpy – phase changes

- Enthalpy is very handy for phase changes, because $p$ and $T$ are usually constant. ($T$ must be constant)

- Heat of vaporization $\Delta H_{\text{vap}}$: heat required to convert liquid to vapor (gas)
- Also called enthalpy of vaporization (same thing)
Enthalpies of Formation

• A formation reaction produces 1 mol of a chemical substance from the elements in their most stable forms
  – There is a single product with a stoichiometric coefficient of 1.
  – All the starting materials are elements, and each is in its most stable form.
  – Enthalpies of reactions involving gas vary with pressure, so pressures must be specified.
  – Enthalpies of reactions occurring in solution vary with concentration, so concentration must be specified.
Elements – most stable forms?

- This means the naturally occurring form

  Oxygen  \( \text{O}_2 \) (g)
  Carbon  \( \text{C} \) (graphite)
  Iron  \( \text{Fe} \) (s)
  Sodium  \( \text{Na} \) (s)

- By definition the enthalpy of formation of all of these guys is ZERO.
Must specify ‘state’ of system

• For us, state means the T, p, etc.

• Standard temperature and pressure (STP)
  – $T = 273.15 \text{ K}$ and $p = 1 \text{ atm}$
  – Book says 298 K and 1 atm.
    • Technically this is SATP: standard ambient T and p
  – Actually, can use anything, just need to make sure conditions match whatever table you are using

• Indicate STP with °
Hess’s Law

• Enthalpy of formation of methane
  
  \[ \text{C (graphite) + 2H}_2 (g) \rightarrow \text{CH}_4 (g) \]

  The \( \Delta H \) for this reaction, is the \( \Delta H_{\text{formation}} \) of \( \text{CH}_4 \)

• For more complicated reactions, use Hess’s Law
  – the enthalpy change for any overall process is

  \[ \Delta H^\circ_{\text{rxn}} = \sum \text{coeff}_{\text{products}} \Delta H^\circ_{f \text{products}} - \sum \text{coeff}_{\text{products}} \Delta H^\circ_{f \text{reactants}} \]

  set of steps that leads from the starting
Example

- Determine the standard enthalpy change ($\Delta H_{\text{rxn}}$) for

$$C_2H_4 (g) + 3O_2 (g) \rightarrow 2CO_2 (g) + 2H_2O (l)$$

\[
\begin{align*}
C_2H_4 (g) & \rightarrow 2C (s) + 2H_2 (g) & 52.4 \text{ kJ/mol} \\
3O_2 (g) & \rightarrow 3O_2 (g) & 0 \text{ kJ/mol} \\
2C \text{ (graph.)} + 2O_2 (g) & \rightarrow 2CO_2 (g) & -393.5 \text{ kJ/mol} \\
2H_2 (g) + O_2 (g) & \rightarrow 2H_2O (l) & -285.83 \text{ kJ/mol}
\end{align*}
\]

\[
= 2(-393.5) + 2(-285.83) - [1(52.4) + 3(0)]
= -1358.66 - (52.4)
= -1411.1 \text{ kJ (per mole of } C_2H_4 \text{ burned)}
\]
Today

- Go to seminar 4:00 VDW 102

By Monday

- Start Chapt 7
- Work problems in back of Chapt 6
- Start CAPA #10

Remember: You are done with the homework when you understand it!