Book uses $\Delta$ for phase changes and for chemical reactions.

$\Delta H \leftrightarrow$ change in enthalpy $\leftrightarrow$ change in energy at const P

What we're really interested in (?)

CHEMICAL REACTIONS

We now know that if we write:

$$3A + B \rightarrow C + 2D$$

we must specify $P$, $V$, and $T$ for each (products & reactants).

At constant pressure, $q_p = \Delta H$

The reactions in a human body produce about 6000 kJ/day (basic metabolic rate).

8,000 - 12,000 kJ/day with activity (exercise, etc).

Remember that you can add or subtract reactions and their corresponding enthalpies (result of state variables)

\[ \text{Remember from Gen Chem} \]
Temperature Dependence of \( \Delta H \)

We saw before that to get \( \Delta H \) for:

\[
H_2O \ (l \ at \ 50^\circ) \rightarrow H_2O \ (g \ at \ 50^\circ)
\]

We could take:

\[
\begin{align*}
H_2O \ (l \ at \ 50^\circ) & \xrightarrow{\text{heat}} H_2O \ (l \ at \ 100^\circ) \\
\downarrow & \quad \downarrow \\
H_2O \ (g \ at \ 50^\circ) & \xleftarrow{\text{cool}} H_2O \ (g \ at \ 100^\circ)
\end{align*}
\]

Similarly, if we know \( \Delta H \) for \( A \rightarrow B \) at 25\(^\circ\)

to calculate \( \Delta H \) for \( A \rightarrow B \) at 37\(^\circ\)

\[
A \ (37^\circ) \xrightarrow{\text{Cp}} A \ (25^\circ) \xrightarrow{\Delta H} B \ (25^\circ) \xrightarrow{\text{heat}} B \ (37^\circ)
\]

(This assumes that \( \text{Cp}^{(A)} \) and \( \text{Cp}^{(B)} \) are independent of \( T \) over range of 25\(^\circ\) to 37\(^\circ\))
We never care about $H$, but only $\Delta H$.

Convention has that $H=0$ for any/all pure elements in their most stable states at 1 atm.

Standard enthalpy for molecules is:

- the enthalpy of formation of 1 mol of the compound at 1 atm from its component elements at 1 atm formation ($H=0$ for each of them)

We saw in Gen Chem that we can use standard enthalpies of formation of all components of a reaction to get $\Delta H$ for the net reaction.

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**SUMMARY**

1) Heat ($q$) and Work ($w$) are exchanges of energy between system and surroundings.

2) Chemical reactions or phase changes also change the energy of the system (converting chemical energy).

Intermolecular interactions have energy. Bonds require energy.

$A \rightarrow B$ if $\Delta H < 0$ System will release energy to surroundings.
Calculate ΔH for reacting 1 g solid glyeryl glycinic with O₂ to form solid urea, CO₂ (g) & H₂O (l) at 25°C, 1 atm (isothermal, isobaric).

\[ 3 \text{O}_2 (g) + \text{C}_4\text{H}_8\text{N}_2\text{O}_3 (s) \rightarrow \text{CH}_4\text{N}_2\text{O} (s) + 3\text{CO}_2 (g) + 2\text{H}_2\text{O} (l) \]

\[ \Delta H^\circ_{\text{Rxn}} = \bar{H}^\circ (\text{urea}) + 3\bar{H}^\circ (\text{CO}_2 (g)) + 2\bar{H}^\circ (\text{H}_2\text{O}, l) - \bar{H}^\circ (\text{C}_4\text{H}_8\text{N}_2\text{O}_3, s) - 3\bar{H}^\circ (\text{O}_2, g) \]

\[ = -333.17 \text{ kJ/mol} + 3(-393.51 \text{ kJ/mol}) + 2(-285.83 \text{ kJ/mol}) - (-745.25 \text{ kJ/mol}) - 3(0) \]

\[ = -1340.11 \text{ kJ/mol} \]

Heat is taken from system i.e. is given off

Then \((-1340.11 \text{ kJ/mol}) \times \left(\frac{1 \text{ mol}}{132.12 \text{ g}}\right) = -10.14 \text{ kJ g}^{-1}\)

What about doing this at a non-standard temp?

\(\bar{H}^\circ\) really means \(\bar{H}^\circ_{298}\)

But from eq. 2.44

\[ \Delta H(T_2) = \Delta H(T_1) + \Delta C_p (T_2 - T_1) \]

\[ \bar{H}^\circ_T = \bar{H}^\circ + \Delta C_p (T - 298) \]

\(\Delta C_p = ?\)

An example of breaking 1 process into 2 steps
What about other pressures?

For ideal gases, $H$ is independent of $P$.
For solids & liquids, $H$ depends weakly on $P$ (usually).

So often can use $H^\circ$ at $P = 1$ atm.

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**Bond Dissociation Energies (Enthalpies)**

$$A-B (g) \rightarrow A(g) + B(g)$$  
Should be measure of energy required to break bond $A-B$

Used in Organic texts to get a feel for molecule stability.

$$\text{CH}_3-H (g) \rightarrow \text{CH}_3 (g) + H^-(g)$$  
$$\Delta H \approx 415 \text{kJ/mol}$$  
\text{ie. for C-H bond generically.}  
(Not absolute, but often OK...)

$$\text{CH}_3-\text{CH}_2-H (g) \rightarrow \text{CH}_3-\text{CH}_2^-(g) + H^-(g)$$

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**SUMMARY:**

For an ideal gas, the internal energy is a direct measure of temperature.
Which is kinetic energy (and rotational).

Raise $T$, raise kinetic energy (billiard balls).
Real gases, liquids, solids

\[ \text{translational, rotational, vibrational } E \text{'s plus interactions between molecules} \]

\[ \text{Compress} \]

We have all the energetic considerations for an ideal gas.

\[ \text{Plus if the molecules repel each other, we have to put in extra energy to make up for increased repulsion as molecules get closer (on average).} \]

Conversely, if the molecules attract each other, it ought to be easier to compress the gas.

Real heat capacities reflect this.

Chemical reactions (and phase changes) release or absorb large amounts of energy.
Auto Engine

Assume for simplicity that the gas in piston is isolated (no heat xfer w/ surroundings - adiabatic).

We know not true - why?

Assess Reversible or Irreversible?

Initially, V unchanged, \( P = \frac{nRT}{V} \) \( \text{const} \)

So \( P \) increases dramatically. Pressures no longer balanced, so volume changes.

Less obvious, but cells "carry out" reactions which result in work (electrical, DNA, etc.) and heat.

Exercise science and physiologists can tell us all about this!