

Unit 3, Lesson 09: Estimating ΔH Using Bond Energies

Enthalpy is essentially the total chemical potential energy (or internal energy) of a substance.

Chemical potential energy is found in a substance three ways:

- as electrostatic attraction between an atom's nucleus and its electrons
- as inter-molecular forces of attraction between molecules of the substance
- as intra-molecular forces of attraction (chemical bonds) between the atoms within each molecule

It is the chemical potential energy of the bonds that is responsible for most of the change in enthalpy (ΔH) during a chemical reaction, so we can use bond energies to estimate ΔH for a reaction.

Bond energy: (aka bond dissociation energy) is the amount of energy that is **required** to break a chemical bond

- breaking bonds always requires energy
- forming bonds always releases energy

Average bond energies for some common bonds are given on page 599 of your text.

We can visualize chemical reactions as happening as two steps:

- the bonds in the reactants are broken (which requires energy) to form free atoms
- the free atoms bonds to form the products (which releases energy)

The enthalpy change of a reaction is approximately equal to the difference in the energy required to break the bonds of the reactants and the energy given off when the bonds in the products are formed:

$$\Delta H = \sum \text{bond energy of reactants} - \sum \text{bond energy of products}$$

eg. Use bond energies to estimate ΔH for: $2 \text{H}_2 (\text{g}) + \text{O}_2 (\text{g}) \rightarrow 2 \text{H}_2\text{O} (\text{g})$

Bonds in reactants that are broken:	2 (H – H) bonds	requires	2 (436 kJ) = 872 kJ
	1 (O = O) bond	requires	1 (498 kJ) = <u>498 kJ</u>
			1370 kJ

Bonds in products that are formed:	4 (O – H) bonds	releases	4 (460 kJ) = 1840 kJ
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$$\Delta H = \sum \text{bond energy of reactants} - \sum \text{bond energy of products}$$

$$= 1370 \text{ kJ} - 1840 \text{ kJ}$$

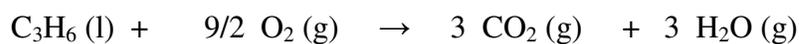
$$= -470 \text{ kJ for 2 moles of H}_2\text{O or } -235 \text{ kJ/mol of water vapour formed}$$

(this is very close to the actual molar enthalpy of formation of water vapour, -241.8 kJ/mol)

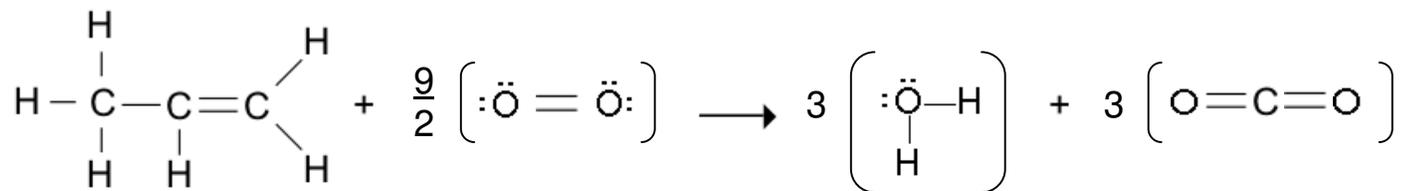
Caution: be careful that you are using the correct structural formulas for compounds when you are determining what number of each type of bond is in each molecules. You need to remember how to draw the structures from the organic chemistry unit:)

eg. Calculate ΔH for the combustion of propene using bond energies.

Step 1: Write the combustion equation for propene



It may help to draw the structural formulas for the molecules before you count the bonds:



Step 2: substitute into the equation to find ΔH using bond energies

$$\Delta H = \sum \text{bond energy of reactants} - \sum \text{bond energy of products}$$

$$= [1 (\text{C}-\text{C}) + 1 (\text{C}=\text{C}) + 6 (\text{C}-\text{H}) + \frac{9}{2} (\text{O}=\text{O})] - [6 (\text{H}-\text{O}) + 6 (\text{C}=\text{O})]$$

$$= [347 \text{ kJ} + 607 \text{ kJ} + 6(338 \text{ kJ}) + (\frac{9}{2} (498\text{kJ}))] - [6 (460 \text{ kJ}) + 6 (745 \text{ kJ})]$$

$$= 5223 \text{ kJ} - 7230 \text{ kJ}$$

$$= -2007 \text{ kJ}$$

Step 3: “sanity test” Does your answer make sense?

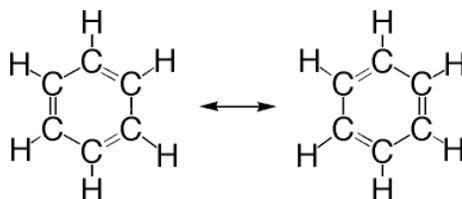
Yes. This is a combustion reaction for a hydrocarbon, so the ΔH should be large and negative.

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Homework:

1. Read pages 226 to 229 in McGraw-Hill, on physical and nuclear changes
2. Use bond energies to estimate the heat of reaction (ΔH) for the following:
 - a) $C_5H_8 + 2 H_2 \rightarrow C_5H_{12}$ (C_5H_8 is 1,3-pentadiene)
 - b) $C_2H_5OH + 3 O_2 \rightarrow 2 CO_2 + 3 H_2O$
 - c) $C_3H_4 + 2 Cl_2 \rightarrow C_3H_4Cl_4$ (C_3H_4 is cyclopropene)
 - d) the complete combustion of butane
 - e) $2 NH_3 + 3 HOCl \rightarrow N_2 + 3 H_2O + 3 HCl$

3. The bonding in benzene is unusual. While the structure is often shown with alternating single and double bonds around the carbon ring, evidence shows that all six bonds are the same and are neither single nor double bonds.



The complete combustion of benzene produces 3260 kJ of energy per mole of benzene burned.

Use bond energies to “work backward” to calculate the average bond energy of the six carbon-carbon bonds in benzene. What does the value suggest about the “nature” of these bonds?

Answers:

2a) $\Delta H = + 40 \text{ kJ}$

2b) $\Delta H = - 1391 \text{ kJ}$

2c) $\Delta H = + 112 \text{ kJ}$

2d) $\Delta H = - 2902 \text{ kJ}$

2e) $\Delta H = - 780 \text{ kJ}$

3. The BE of the carbon-carbon bond in benzene is + 446 kJ. This is half-way in between the BE for C – C and C = C bonds, and supports the idea that the carbon-carbon bond in benzene is a resonance structure and is like a 1 ½ bond)