ESTIMATING THE ENTHALPY CHANGE FOR A REACTION USING AVERAGE BOND ENERGIES

The energy change (enthalpy change) that occurs during a chemical reaction results from the breaking and forming of bonds. The breaking of a bond requires energy to be absorbed (endothermic). The forming of a bond releases energy (exothermic). The enthalpy change for a reaction is the sum of all these energy changes associated with the breaking and forming of bonds.

If the energy absorbed to break bonds is greater than the energy released by the formation of bonds then the reaction is endothermic (ΔH is positive).

If the energy absorbed to break bonds is less than the energy released by the formation of bonds then the reaction is exothermic (ΔH is negative).

We can estimate the enthalpy change for a reaction by imagining all the bonds breaking in the reactants and then all the bonds forming in the products, and calculating the sum of all these energy changes. (Note that this is not what really happens in most chemical reactions but the result is valid as long as we start with the correct reactants and end with the correct products. The energy change does not depend on how we get from one to the other.)

<u>Example</u>

Use bond energies to estimate the molar enthalpy change for the complete combustion of acetylene.

1. Write the balanced chemical equation.

   $2\ C_2H_2(g)\ +\ 5\ O_2(g)\ \rightarrow\ 4\ CO_2(g)\ +\ 2\ H_2O(g)$

   You may need to write out the structures to be clear on what bonds are breaking and forming.

   2 H−C≡C−H + **5** O=O → **4** O=C=O + **2** H−O−H

2. Determine the amounts of bonds broken and formed, and the associated enthalpy changes.

   Bonds Breaking

BOND	AMOUNT OF BONDS BROKEN IN THE REACTANTS	ENTHALPY CHANGE This is the positive value of the bond dissociation energy from the table.
H−C	4 mol (2 moles of acetylene molecules × 2 H−C bonds per molecule)	+413 kJ/mol
C≡C	2 mol (2 moles of acetylene molecules × 1 C≡C bond per molecule)	+839 kJ/mol
O=O	5 mol (5 moles of oxygen molecules × 1 O=O bond per molecule)	+495 kJ/mol

   Bonds Forming

BOND	AMOUNT OF BONDS FORMED IN THE PRODUCTS	ENTHALPY CHANGE This is the negative value of the bond dissociation energy from the table.
C=O	8 mol (4 moles of carbon dioxide molecules × 2 C=O bonds per molecule)	–799 kJ/mol
H−O	4 mol (2 moles of water molecules × 2 H−O bonds per molecule)	–467 kJ/mol

3. Calculate the sum of all the enthalpy changes. (Note that this calculation is an estimate of enthalpy because we are using <u>average</u> bond energies.)

$$\Delta H \approx 4\ \cancel{mol}(+413\ kJ/\cancel{mol}) + 2\ \cancel{mol}(+839\ kJ/\cancel{mol}) + 5\ \cancel{mol}(+495\ kJ/\cancel{mol}) + 8\ \cancel{mol}(-799\ kJ/\cancel{mol}) + 4\ \cancel{mol}(-467\ kJ/\cancel{mol})$$

$$= -2455\ kJ$$

4. The question asks for the molar enthalpy change so we must do one more step.

$$\Delta H_{COMBUSTION} = \frac{\Delta H}{n_{C2H2}} = \frac{-2455\ kJ}{2\ mol} = -1227.5\ kJ/mol$$

(2 mol of C_2H_2 in the chemical equation used to calculate ΔH)

   Therefore, the molar enthalpy change for the combustion of acetylene is –1228 kJ/mol.