

ICT: Thermodynamics: Use of a Spreadsheet — Bond Enthalpies

SCH4UE_08 - 09

The enthalpy change of combustion of a compound can be found from bond enthalpies.

The energy needed to break the bonds in the reactants is firstly determined, (the process of breaking bonds in a molecule is always endothermic); and then all the energy released when the new bonds are made in the products is determined, (the formation of bonds from atoms or radicals in the gas phase is always exothermic).

Thus, the standard enthalpy of reaction is the difference between the sum of the average standard bond enthalpies of the products and the sum of the average standard bond enthalpies of the reactants:

$$\Delta H^{\circ}_{\text{Reaction}} = \Sigma D(\text{bonds broken}) - \Sigma D(\text{bonds formed})$$

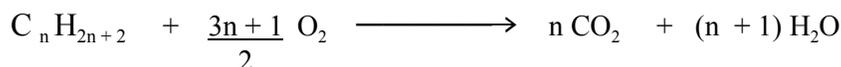
This equation tells you to multiply the bond energy for each bond broken by the number of bonds of that type, and add all of these up. Then, multiply the bond energy for each bond formed by the number of bonds of that type, and add all of these up.

Because bond formation is exothermic, the quantity “ $\Sigma D(\text{bonds formed})$ ” is subtracted from the quantity “ $\Sigma D(\text{bonds broken})$.”

The same standard calculation is performed to determine the enthalpy change of combustion of any compound. Hence, it is quite easy to set up a standard spreadsheet to do the calculation.

Construct a standard spreadsheet for a series of alkane fuels (general formula $C_n H_{2n+2}$).
[Note: when $n = 1$, methane, CH_4 ; $n = 2$, ethane; etc.)

1. Construct a spreadsheet to calculate the enthalpy changes of combustion of alkanes. The enthalpy change of combustion for any non-cyclic alkane may be determined using the following equation:



2. Use your spreadsheet to calculate the enthalpy change of combustion for the series of straight-chain alkanes methane to nonane. Use Table 10: Average Bond Enthalpies of the Data Book.
3. Plot a graph of enthalpy change of combustion against number of carbon atoms in the chain.
4. Compare the values you calculated using Table 10 with those in Table 12: Enthalpies of Combustion in the Data Book. Comment on the differences. How can bond enthalpies be used to explain the shape of the graph?
5. Adapt the spreadsheet so that it can calculate the enthalpy change of combustion for alcohols, (general formula $C_n H_{2n+1} OH$), instead of alkanes. Perform the calculations for methanol, CH_3OH , to hexanol, $C_6H_{13}OH$.
(You will need to start with writing a general equation for their combustion.)