

Computational Study of Heats of Formation and Combustion of Hydrocarbons: Pre-Lab Assignment

(This is copied from the handout – you don't need to do prelab twice! This week, the pre-lab assignment will be part of your lab notebook and not turned in separately.)

1. Read the section on thermochemistry in the text in preparation (McQuarrie and Simon 19-10, 19-11).
2. Write out the equation for an example hydrocarbon combustion reaction (balance the equations so 1 mol of hydrocarbon is combusted). Indicate the quantities you will have to compute to determine the heat of combustion from the WebMO calculations.
3. Look up the gas phase heats of formation for each of the compounds below (and your 3 additional compounds) and tabulate them so that we have a reference point for our calculations. The NIST webbook, <http://webbook.nist.gov/chemistry/> is a good source.
4. Set up your laboratory notebook with a title a short description of what we are trying to accomplish in the investigation as well as a general equation for combustion. Include the data from Item 3 above (i.e., heats of formation) in a table.

Compounds

Ethylene	ethanol	Naphthalene	“Kerosene” C ₁₁ H ₂₄
Benzene	methanol	Anthracene	“Octane” n-C ₈ H ₁₈
Toluene	butanol	Phenathrene	Pyrene