

Homework 5A: Enthalpy of Reaction
Due Friday 2/8/08
Chemistry 456, Chapter 4, Written by Lewis Johnson

Our industrial civilization requires a massive amount of energy to function, with the majority of this energy generated by burning fossil fuels. In this assignment, you will use the principles you learned in Chapter 4 to compare the energy content of two different fossil fuels (methane and n-octane), plus two alternative fuels (methane and ethanol), that can be produced through a variety of methods.

Note: This assignment involves a lot of numerical calculations. Use of a calculator or spreadsheet is acceptable, but make sure to show sample calculations involving, at minimum, all symbolic rearrangements of equations, symbolic integration/differentiation, and all unit conversions. Make sure all of your equations are balanced.

All of the Shomate parameters you need for this assignment are given in a table at the end of the assignment, along with the enthalpy of formation values you should use.

Question 1a: Calculate the molar enthalpy of combustion for methane at 298K and 600K using Equation 4.23 in your textbook. Cp values for the compounds are given by the following five-parameter equation known as the Shomate Equation, where $t = T(K)/1000$. (See Table below).

$$C_p^\circ(t) = A + Bt + Ct^2 + Dt^3 + \frac{E}{t^2}$$

Question 1b: Repeat this calculation for combustion of hydrogen at 298K and 600K, using the Shomate form of the heat capacity. *Note that the enthalpy of formation of the most stable form of an element at a temperature other than 298K is not necessarily zero.*

Question 2: Calculate the enthalpy of combustion for n-octane and ethanol at 298K. Then, using all four of your values for enthalpy of combustion at 298K, calculate the energy density of all four fuels in both kJ/kg and kJ/L. Discuss any implications you think these energy densities may have for use of any of these fuels.

Question 3: To put the numbers from above in perspective, make the following two comparisons:

- a) Calculate how many hours of sunlight falling on 1 square meter would be needed to equal the enthalpy of combustion of 1 liter of each of these fuels in their standard state. Note

that mean peak solar flux is typically about 1kW/m^2 , and that Seattle gets the equivalent of 4 hours of mean peak solar flux per day.

- b) Calculate the number of miles per gallon a car with an engine that generates 200 horsepower of useful work from a 50% efficient Otto cycle (hint: The Otto cycle will be covered next chapter, but you don't need to know anything about it for this problem. All numbers you need are given in the assignment.), that is burning n-octane and traveling at 100 km/h. Compare this with a calculation of the same engine burning pure ethanol. Use your enthalpy values at 298K—while not the most accurate, this is just intended to give you a back-of-the envelope estimate—no need to make any temperature corrections.

Note: Car engines typically don't run at anywhere near their maximum output, as can be ascertained by looking at the position of the tachometer needle relative to the redline. Realistically, the car would be running at about 25% of peak output.

Useful conversion factors:

$$1\text{W} = 1\text{ J/s}$$

$$1\text{HP} = 750\text{W}$$

$$1\text{ gallon} = 3.8\text{L}$$

$$1\text{ mile} = 1.6\text{ km}$$

Data Tables:

Shomate Parameters (for use with reduced temperature $t=T/1000$, yield C_p in J/mol K):

Compound	A	B	C	D	E
CO ₂	25	55	-34	8	-0.1
H ₂ O	30	7	7	-3	0.1
O ₂	30	6	-1	0.1	-0.2
H ₂	33	-11	11	-3	-0.2
CH ₄	-1	109	-42	6	0.7

Heats of Formation at 298K:

Compound	ΔH_f^0 (kJ/mol)
CO ₂	-394
H ₂ O	-242
O ₂	0
H ₂	0
CH ₄	-75
C ₂ H ₅ OH	-235
n- C ₈ H ₁₈	-208

Molar weights and densities:

Compound	MW (g/mol)	Density (kg/L)
H ₂	2	0.0001
CH ₄	16	0.4
C ₂ H ₅ OH	46	0.8
n- C ₈ H ₁₈	114	0.7