ENGR 1130 Project D: Fuels and Coolants: Thermochemistry

25 Points See Grading Rubric in Canvas

Why is my teacher having me do this project??

A. To practice Thermochemistry Calculations for chemical reactions. (Module 9)

B. To practice phase change calculations using heats of vaporization and fusion and heat capacities. (M9)

C. To develop an understanding of properties thermodynamically conducive to fuels and coolants. (Module 9)

You have been assigned a compound from the chart posted on the Project D Page in Canvas. You must do the compound you are assigned. This is the same compound you were assigned in Project C (Parts C and D). Yea! The Lewis Structure is done!

*****Clearly show all calculations and go into detail to receive maximum points on this project.**

Part A: Calculating ΔH^o_{rxn} from heats of formation

1. Write the balanced chemical equation for the combustion of your compound. From the equation and the values from Appendix G of your text, calculate the ΔH^o for this reaction (assume standard conditions).

- You will probably need to research the ΔH_f^o for your particular compound. At the end of this document are some good sites with comprehensive thermochemical data.
    - If your compound has nitrogen in it, please add nitrogen gas (is it a HOFBrINCl?) to the products.
    - If your compound has chlorine or fluorine in it, please add these elemental gases (are they HOFBrINCl?) to the products.

Balanced chemical reaction

$$C_6H_{6(gas)} + 7\frac{1}{2}O_{2(gas)} \rightarrow 6CO_{2(gas)} + 3H_2O_{(vap)}$$

$$C_6H_{6(gas)} + 7\frac{1}{2}O_{2(gas)} \rightarrow 6CO_{2(gas)} + 3H_2O_{(liq)}$$

For estimation of heat of reaction for complete combustion, we have two approaches. In one approach, water is considered in vapor phase and not condensed and the heat of reaction in this case is called lower heating value. In second approach, water vapors are considered condensed liquid, and heat of reaction in this case is called higher heating value.

$$C_6H_6(g) + 7\frac{1}{2}O_2(g) \rightarrow 6CO_2(g) + 3H_2O(l)$$

From Appendix G, heat of formation information obtained and tabulated below:

Component	Heat of Formation
C_6H_6	**82.927**
CO_2	**-393.51**
H_2O	**-285.83**
O_2	**0**

Reference temperature is 298 K or 25 degree Celcius.

$$C_6H_6(g)+7\frac{1}{2}O_2(g)\rightarrow 6CO_2(g)+3H_2O(l)$$
$$\Delta H_{rxn}=\sum \Delta H_f^{o}(\text{Products})-\sum \Delta H_f^{o}(\text{Reactants})$$
$$\sum \Delta H_f^{o}(\text{Products})=6mol\times -393.51kJ/mol+3mol\times -285.83kJ/mol$$
$$=-2361.06-857.49=-3218.55$$
$$\sum \Delta H_f^{o}(\text{Reactants})=1mol\times 82.927kJ/mol=82.92$$
$$\Delta H_{rxn}=-3135.623kJ/mol$$

Negative sign shows that it is an exothermic reaction.

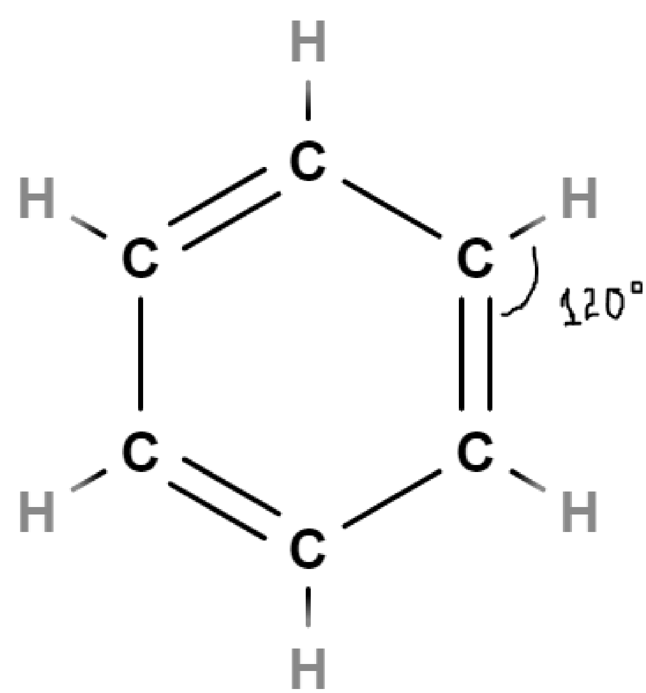
Part B: Calculating ΔH^{o}_{rxn} from bond dissociation energies.

2. Rewrite the balanced chemical equation from Part A, drawing the Lewis structures of all the compounds involved instead of just writing the formulas.

$$C_6H_6(g)+7\frac{1}{2}O_2(g)\rightarrow 6CO_2(g)+3H_2O(l)$$

- Create a Bonds Broken and Bonds Formed table and record your data. (See the Example below)

Type of Bond Broken (Reactant Bonds)	Quantity of Bond Type	Type of Bond Formed (Product Bonds)	Quantity of Bond type
C-H	1x3	C=O	6x2
C=C	1x3	H-O	3x2
O=O	7.5x1		



3. Using the Bond Energies, calculate the ΔH^o_{rxn} for the combustion reaction. You can find a chart of Bond Dissociation Energies in Section 7.5 (Tables 7.2 and 7.3) of your text. Section 7.5 also has some examples of this type of calculation.

- Clearly show your work. It may be easier to show your work by modifying your chart in 2 (adding in the bond energy values and the total ΔH from each compound)
- $\Delta H^o rxn = \Sigma D(\text{bonds broken}) - \Sigma D(\text{bonds formed})$
- If you have significant differences, which calculation do you think is more accurate?

$$\Delta H^o rxn = \sum SD(bonds\ broken) - \sum SD(bonds\ formed)$$
$$H-H = 436kJ/mol$$
$$H-C = 415kJ/mol$$
$$H-O = 464kJ/mol$$
$$C-C = 345kJ/mol$$
$$C=C = 611kJ/mol$$
$$C=O = 741kJ/mol$$
$$O=O = 498kJ/mol$$
$$\sum SD(bonds\ broken) = 3x415 + 611x3 + 7.5x498 = 6813kJ$$
$$\sum SD(bonds\ formed) = 6x2x741 + 3x2x464 = 11676kJ$$
$$\Delta H^o rxn = \sum SD(bonds\ broken) - \sum SD(bonds\ formed)$$
$$= 6813kJ - 11676kJ = -4863kJ$$

C-H	1x3x415 kJ	C=O	6x2x741 kJ
C=C	1x3=611x3 kJ	H-O	3x2x464 kJ
O=O	7.5x1 = 7.5x498 kJ		

Bond formed in products are stronger than those present in reactant so excess energy is released. As bond energies present in the table are basically average values of bond energy, so it gives only a rough estimate of the heat of reaction or enthalpy change. The answer obtained by heat of formation method is more accurate as compared to method utilizing bond energies. So, answer obtained from heat of formation method is more accurate.

Bond Energies (kJ/mol)

Bond	Bond Energy		Bond	Bond Energy		Bond	Bond Energy
H–H	436		C–S	260		F–Cl	255
H–C	415		C–Cl	330		F–Br	235
H–N	390		C–Br	275		Si–Si	230
H–O	464		C–I	240		Si–P	215
H–F	569		N–N	160		Si–S	225
H–Si	395		$N = N$	418		Si–Cl	359
H–P	320		$N \equiv N$	946		Si–Br	290
H–S	340		N–O	200		Si–I	215
H–Cl	432		N–F	270		P–P	215

Table 7.2

Average Bond Lengths and Bond Energies for Some Common Bonds

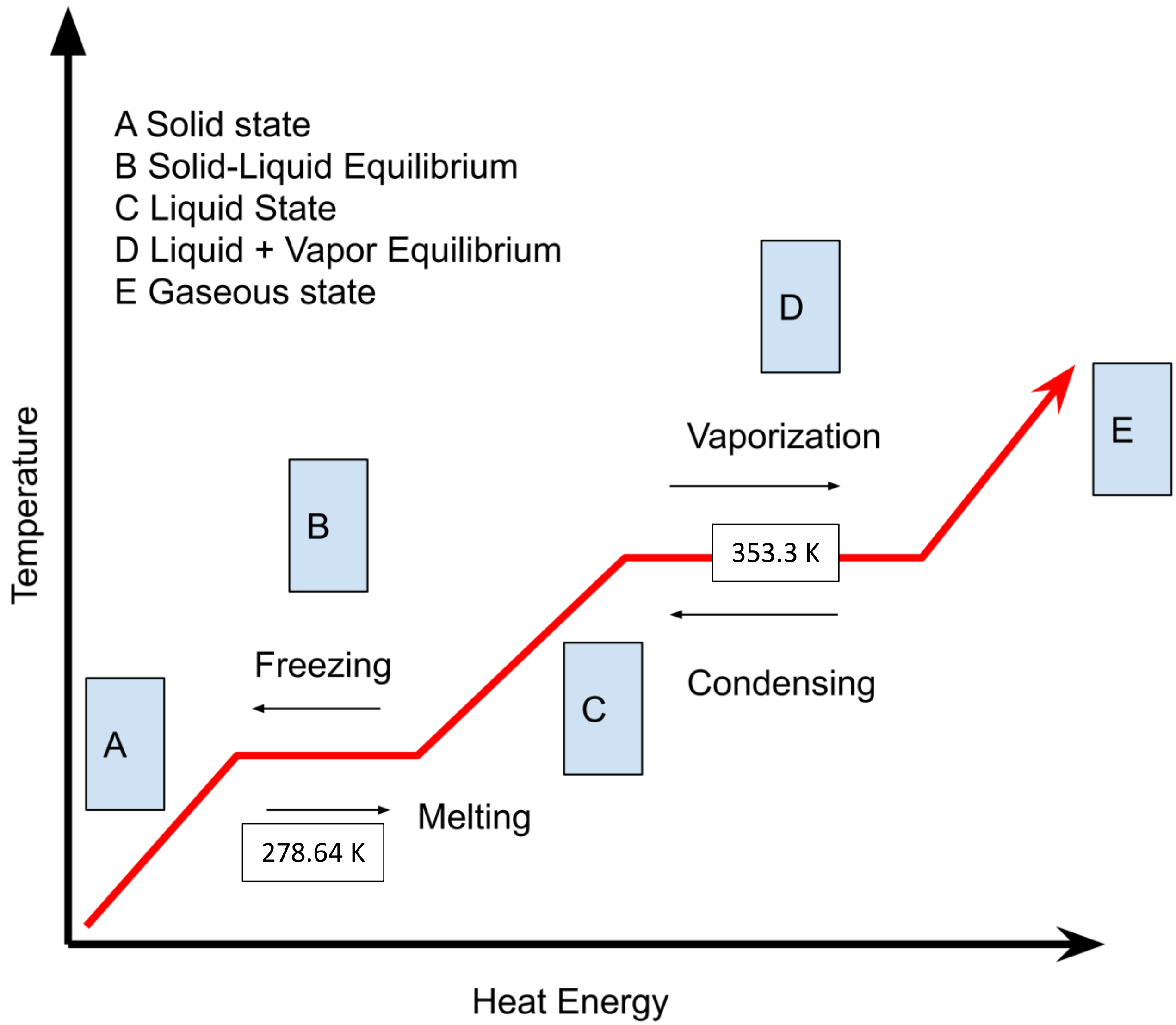
Bond	Bond Length (Å)	Bond Energy (kJ/mol)
C–C	1.54	345
$C = C$	1.34	611
$C \equiv C$	1.20	837
C–N	1.43	290
$C = N$	1.38	615
$C \equiv N$	1.16	891
C–O	1.43	350
$C = O$	1.23	741
$C \equiv O$	1.13	1080

Table 7.3

4. Compare the values from Parts A and B. Try to account for any differences.

Part C: Phase Change Diagrams and Calculation

5. Draw a phase change diagram (like the one below) labeling the temperatures at which the phase changes occur. Do not copy this diagram, create your own. On your diagram indicate what is happening at each part (letters A, B, C, D, E)—like what phase change (verb) and what states of matter are present.



6. Research the heats of fusion and vaporization for your compound. Calculate the amount of energy needed to convert 1 kilogram of your substance from the solid phase all the way to the gas phase. (Choose a starting temperature below the melting point and an ending temperature higher than the boiling point.)

Starting temperature = 273 K
Fusion Temperature =278.64 K
Boiling Temperature =353.3 K

Q required = Cpsolid*(Tfusion-Tstart) + lambda_fusion + Cpliquid*(Tboiling-Tfusion)+lambda_boiling =
= (278.64-273)*47.86/1000+9.68+(353.3-278.64)*135.69/1000+30.72=0.269+9.68+10.13+30.72=50.799 kJ/mol
= 50.799 kJ/mol*1m0/0.078kg=651.27 kJ/kg

Part D: Compound Analysis

7. Would your compound be a good choice to be used as a fuel? rocket fuel? airplane fuel?
   - Using your value from Part A—determine the energy density of your compound. (kJ/gram)
   - How does this energy density compare to other fuels?
     - Choose two commonly used fuels and compare.

3135.62 kJ/mol*1mol/0.078kg = 40.2 MJ/kg or energy density of Benzene or 40.2 kJ/gram.
Gasoline Energy density = 46.4 MJ/kg
Jet fuel = 43 MJ/kg
It is already being used as a fuel additive and is not usually utilized as fuel due to its toxic nature and storage problem.

8. Would your compound be a good choice to be used as a coolant? Why or why not?
   - Use your work from Part C to support your answer.
   - Compare your compound to two typical coolants. How do your compound's properties compare to common coolants?
   - What are qualities of "good" coolants?
   - In what engineering applications are coolants needed/used?

Liquid heat capacity is 1.74 kJ/kgK which is quite low as compared to water and its boiling point is below boiling point of water. So, it is not recommended as coolant.
Water is universal coolant as it has large heat capacity and also heat of vaporization.

Part E: Citations

https://webbook.nist.gov/cgi/cbook.cgi?ID=C71432&Mask=1#Thermo-Gas
https://webbook.nist.gov/cgi/cbook.cgi?ID=C71432&Mask=4#Thermo-Phase
https://en.wikipedia.org/wiki/Energy_density

Websites for finding good thermochemical data.
National Institute of Standards and Technology: [NIST Chemistry WebBook]
Organic Compounds: [Physical and Thermochemical Data]
NIH National Library of Medicine: [PubChem]