Chem 231 **Assignment #4** (due Tuesday, 27 October, in class)

1. [2] Graphite and diamond are well-known allotropic forms of carbon. Buckminsterfullerene, C_{60}, a remarkable allotrope of carbon consisting of molecules of sixty icosahedrally-bonded carbon atoms, was discovered in 1985. Briefly describe how the standard enthalpy of formation of buckminsterfullerene could be measured.

2. [2] Calculate the standard enthalpy change at 25 °C for

a) the combustion of phenol: $C_6H_5OH(s) + 7O_2(g) = 6CO_2(g) + 3H_2O(l)$

b) the combustion of methane: $CH_4(g) + 2O_2(g) = CO_2(g) + 2H_2O(l)$

Data at 25 °C:
$\Delta H_{fm}°(C_6H_5OH,s) = -165.0$ kJ mol^{-1}
$\Delta H_{fm}°(CH_4,g) = -74.8$ kJ mol^{-1}
$\Delta H_{fm}°(CO_2,g) = -393.5$ kJ mol^{-1}
$\Delta H_{fm}°(H_2O,l) = -285.8$ kJ mol^{-1}

3. [4] **a)** Burning fossil fuels such as coal, petroleum and natural gas, releases CO_2 into the atmosphere. The increasing levels of atmospheric CO_2 causes global warming. How?

b) Coal is a complex and highly variable mineral consisting of partially oxidized aromatics and many other compounds. The standard enthalpy of combustion of coal is roughly equal to that of phenol. Use this approximation to calculate the number of moles of phenol that must be burned to produce 1.00 MJ of heat at 25 °C and 1.00 bar. Also calculate the number of moles of CO_2 produced.

c) Assuming natural gas is pure methane, an good approximation here, calculate number of moles of methane that must be burned to produce 1.00 MJ of heat at 25 °C and 1.00 bar. Also calculate the number of moles of CO_2 produced.

d) To minimize global warming, which is a better fuel, coal or natural gas? Explain.

4. [3] Calculate the standard change in the internal energy ($\Delta U°$) for the formation of 1.00 mole of deuterium molecules from atomic deuterium: $D(g) + D(g) = D_2(g)$.

Data: $\Delta H_{fm}°(D, g) = 218$ kJ mol^{-1}

5. [2] Thermodynamics applies to nuclear reactions too! Using Einstein's famous equation $U = mc^2$, calculate the standard change in the internal energy for the formation of 1.00 mol of helium by the nuclear fusion of deuterium: $D(g) + D(g) = He(g)$. *Hint*: $\Delta U = c^2\Delta m$, where c is the speed of light (2.998×10^8 m s^{-1}) and Δm is the change in mass.

Data: $M_D = 2.013506148$ g mol^{-1} $M_{He} = 4.001412584$ g mol^{-1}

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6. Multi-billion dollar international research projects, such as **ITER** in Europe and **NIF** in the United States, are underway to develop nuclear fusion for commercial energy production. Give

[2] two important advantages of nuclear fusion as an energy source over fossil fuels.

ITER (International Thermonuclear Fusion Experimental Research), *see*: https://www.iter.org/

NIF (National Ignition Facility), *see*: https://lasers.llnl.gov/

7. Magnesium is burned in flares and fireworks to produce very high temperatures and intense white light. Magnesium initially at 25 °C is burned adiabatically in pure oxygen.

[3] $$Mg(s) + \tfrac{1}{2} O_2(g) = MgO(s)$$

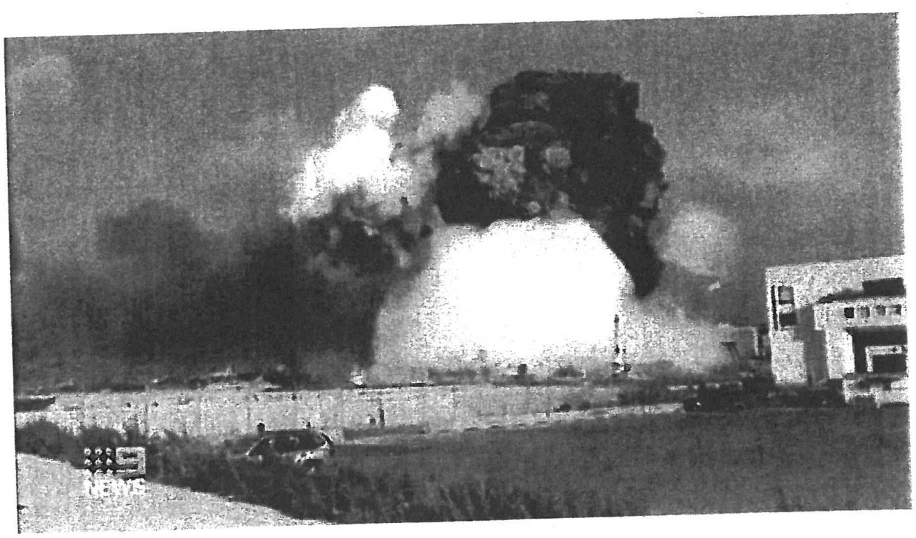
Estimate the final temperature. *Hint*: Use the heat released by the combustion reaction at 25 °C to heat up the MgO(s) reaction product.

Data at 25 °C: $\Delta H_{fm}°(MgO,s) = -601.7$ kJ mol^{-1} $C_{pm}°(MgO,s) = 37.2$ J K^{-1} mol^{-1}

8. Prove $(\partial H/\partial p)_T = 0$ for an ideal gas. [1]

9. Several thousand kilograms of ammonium nitrate fertilizer exploded in Beirut Harbor on 4 August 2020, causing many fatalities and severe damage to the city. The massive blast produced a rapidly-expanding hemispherical white cloud, that quickly disappeared, followed by a huge

[1] column of reddish-brown gas. NO_2 from the ammonium nitrate decomposition causes the reddish-brown color, but what caused the transient white cloud?



See: https://www.youtube.com/watch?v=-OvgHZM95C0

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(Q1) How to measure the standard enthalpy of formation of buckminsterfullerene (C_{60})?

measure the enthalpy change for burning C_{60}:

$$C_{60}(s) + 60\,O_2(g) \rightarrow 60\,CO_2(g) \qquad \Delta H_1$$

the reverse reaction:

$$60\,CO_2(g) \rightarrow 60\,O_2(g) + C_{60}(s) \qquad -\Delta H_1$$

add to:

$$60\,C(\text{graphite}, s) + 60\,O_2(g) \rightarrow 60\,CO_2(g) \qquad \Delta H = 60\,\Delta H_{fm}(CO_2)$$

$$60\,C(\text{graphite}, s) \rightarrow C_{60}(s) \qquad \Delta H_{fm}(C_{60}, s)$$

using "thermochemical algebra":

(easily measured) (accurately known)

$$\Delta H_{fm}(C_{60}, s) = -\Delta H_1 (\text{for } C_{60} \text{ combustion}) + 60\,\Delta H_{m,\text{combust}}(C, \ldots)$$

$$= \boxed{60\,\Delta H_{m,\text{combustion}}(C, gr) - \Delta H_{m,\text{combustion}}(C, C_{60})}$$

a similar procedure was illustrated in class to calculate the standard enthalpy of formation of diamond, another carbon allotrope:

$$\Delta H_{fm}(C, \text{diamond}) = \Delta H_{m,\text{combustion}}(C, \text{graphite}) - \Delta H_{m,\text{combustion}}(C, \text{diamond})$$

Q2 a) standard enthalpy change for phenol combustion:

$$C_6H_5OH(s) + 7O_2(g) \overset{25°C}{=} 6CO_2(g) + 3H_2O(l)$$

$$\Delta H^\circ_{c,m}(C_6H_5OH, s) = \Delta H^\circ_f(\text{products}) - \Delta H^\circ_f(\text{reactants})$$

$$= 6\Delta H^\circ_{fm}(CO_2, g) + 3\Delta H^\circ_{fm}(H_2O, l) - \Delta H^\circ_{fm}(C_6H_5OH, s) - 7\Delta H^\circ_{fm}(O_2, g)$$

$$= 6[-393.5\,kJ] + 3[-285.8\,kJ] - [-165.0\,kJ] - 7[0]$$

$$= \boxed{-3053\ kJ}$$

b) standard enthalpy change for methane combustion:

$$CH_4(g) + 2O_2(g) = CO_2(g) + 2H_2O(l)$$

$$\Delta H^\circ_{c,m}(CH_4, g) = \Delta H^\circ_{fm}(CO_2, g) + 2\Delta H^\circ_{fm}(H_2O, l) - \Delta H^\circ_{fm}(CH_4, g) - 2\Delta H^\circ_{fm}(O_2, g)$$

$$= -393.5\,kJ + 2(-285.8\,kJ) - (-74.8) - 2(0)$$

$$= \boxed{-890.3\ kJ}$$

Q3 a) Burning coal, petroleum, natural gas, wood, etc. produces CO_2 gas, increasing the concentration of CO_2 in the atmosphere.
CO_2 absorbs infrared (heat) radiation, increasing the temperature of the atmosphere

(Q3 cont.) $(1 \text{ MJ} = 10^6 \text{ J})$

b) burning one mole of phenol (~coal) produces 3057 kJ of heat and 6 moles of CO_2.

to produce 1 MJ = 1000 kJ heat:

burn $\frac{1000 \text{ kJ}}{3057 \text{ kJ mol}^{-1}}$ = 0.327 mol phenol

producing 0.327 (6 mol) = **1.96 mol CO_2**

$[C_6H_5OH + 7O_2 \rightarrow 6CO_2 + 3H_2O]$

c) burning one mole of methane produces 890.3 kJ of heat and 1 mole of CO_2.

to produce 1 MJ = 1000 kJ heat:

burn $\frac{1000 \text{ kJ}}{890.3 \text{ kg mol}^{-1}}$ = 1.12 mol methane

producing 1.12 (1 mol) = **1.12 mol CO_2**

$[CH_4 + 2O_2 \rightarrow 1CO_2 + 2H_2O]$

d) To produce a given amount of heat by burning coal or methane (~ natural gas), burning methane produces $\frac{1.12}{1.96}$ = 0.57 (57% of the CO_2 produced by burning coal (methane is the better fuel)

Q4 Calculate the standard energy change ΔU°

for $D(g) + D(g) = D_2(g)$

$$\Delta H^\circ = \Delta H^\circ_{fm}(D_2, g) - 2\Delta H^\circ_{fm}(D, g)$$

$$= 0 - 2(218 \text{ kJ})$$

$$\boxed{\Delta H^\circ = -436 \text{ kJ} = q}$$ (constant pressure here)

work $w = -\int p_{ext}\, dV = -\int p\, dV = -p\int dV$

$$w = -p\Delta V = -p(V_{mD2} - 2V_{mD})$$

$$= -p\left(\frac{RT}{p} - 2\frac{RT}{p}\right) = RT$$

$$= (8.314 \text{ J K}^{-1}\text{mol}^{-1})(298.15 \text{ K})$$

$$\boxed{w = 2480 \text{ J}}$$

Energy change $\boxed{\Delta U = q + w = -433.5 \text{ kJ}}$

Q5 nuclear reaction $D(g) + D(g) = He(g)$

* convert g to kg to get Joules

$$\Delta U = c^2 \Delta m = c^2(M_{He} - 2M_D)$$

$$= (2.998 \times 10^8 \text{ m s}^{-1})^2 [0.004001412584 - 2(0.00201350648)]$$

$$= \boxed{-2.30 \times 10^{12} \text{ J}} = -2.30 \times 10^6 \text{ MJ}$$

$$= -230 \text{ GJ}$$

Q6 Nuclear fusion of deuterium atoms

produces $\frac{2.30 \times 10^{12}\ J}{433.5 \times 10^{3}} = 5.30 \times 10^{6}$

* ≈ 5 million times more energy than the chemical reaction

* No CO_2 produced by fusion energy production.

* Deuterium (and other fusion fuels) are widely available in limitless supply in seawater

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Q7 burn magnesium at 25 °C: ($T_i = 298.15\ K$ (25 °C))

$$Mg(s) + \frac{1}{2} O_2(g) = MgO(s) \quad \Delta H(T_i) = -601.7\ kJ$$

strongly exothermic (lots of heat released) reaction

adiabatic reaction temperature $T_f \approx T_i - \frac{\Delta H(T_i)}{C_p(\text{products})}$

$$T_f = 298.15\ K - \frac{-601700\ J\ mol^{-1}}{37.2\ J\ K^{-1}\ mol^{-1}}$$

$$= 298.15\ K + 16{,}200\ K$$

$$T_f = 16{,}500\ K$$ (that's hot!)

* actual T_f is < 16500 K because C_p increases with T and MgO(s) melts (absorbing heat).

(Q8) For any system (ideal gas, real gas, solids, liquids):

$$\left(\frac{\partial H}{\partial p}\right)_T = V(1-\beta T)$$

for an ideal gas $\beta = \frac{1}{T}$ and

$$\left(\frac{\partial H}{\partial p}\right)_T = V\left(1-\frac{1}{T}T\right) = V(1-1) = 0$$

(Q9) The very fast (almost instantaneous and ∴ adiabatic) explosive decomposition of several thousand tons of ammonium nitrate

$$(NH_4NO_3)_{(s)} \longrightarrow N_2(g),\ H_2O(g),\ NO_2(g)\ \ldots$$

produced a rapidly expanding adiabatic shock wave, cooling the air and condensing water vapor to produce a white cloud of water droplets. Warming of the air after the shock wave passed evaporated the water droplets.