HW5

We can describe enthalpy as H = U + PV, where U – internal energy of the system, P – pressure of the system, V – volume of the system. Since we don't know the absolute value of U for our "chemical" purposes this equation is useless. But we can presume that our system in under constant pressure (pressure does not change), that is true for the most chemical reactions, and then we can calculate the enthalpy change (it is basically heat added or taken out from the system, system in our case is chemical reaction)

What substance is more stable, graphite or diamond?

C (graphite) + O_2 → CO_2 **Δ** H=- 393.8 kJ/mol
C (diamond) + O_2 → CO_2 **Δ** H=- 395.7 kJ/mol

In the reaction with graphite 1 mole of CO_2 is produced and 393.8 kJ of energy is released in the surrounding. In the reaction with diamond 1 mole of CO2 is produced and 395.7 kJ of energy is released. We can presume that diamond has higher energy compare to graphite, so diamond is less stable.

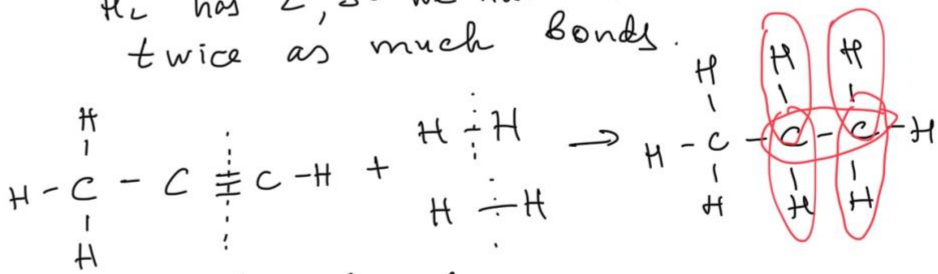
Enthalpy change (**Δ** H) of the reaction – amount of chemical heat energy taken in (giving out) in a reaction. If we know the sign of enthalpy change we can describe if a reaction endothermic or exothermic.

Bond enthalpy: energy required to break 1 mole of a bond.
Let's break C – H bond (ignore all the other bonds that carbon has to have). We need energy to break this bond.
C – H → C. (g) + H. (g)
dot here represents electron, since bond is pair of electrons, when we break the bond, each atom is going to have unpaired electron now.
We will apply 413 kJ of energy to break this bond.
Information about different bond energies (bond enthalpy) can be found in tables online or in textbook. Bond enthalpies can be used to calculate enthalpy change (**Δ** H) of the reaction.

Let's look at the following problem: We need to find the enthalpy change of the reaction only knowing the bond energy of the reactants (C_3H_4 and H_2) and the product(C_3H_8).

$C_3H_4(g) + 2H_2(g) \rightarrow C_3H_8(g)$

remember about coefficient
H_2 has 2, so we have to break
twice as much bonds.



We have to break.

one C≡C bond, bond enthalpy 835 kJ/mol
and two H–H bond, bond enthalpy 436

5 bonds will be formed:
one C – C, bond enthalpy 346
four C – H, 413 kJ/mol

To calculate ΔH of the reaction
we have to subtract energy
of the new bonds from the energy
of the old bonds

ΔH_r = energy of the broken bonds –
energy of the formed bonds

$845 + (2 \cdot 436) - (346 + 4 \cdot 413) =$
$= -291$ $\Delta H_r = -291\ kJ/mol$

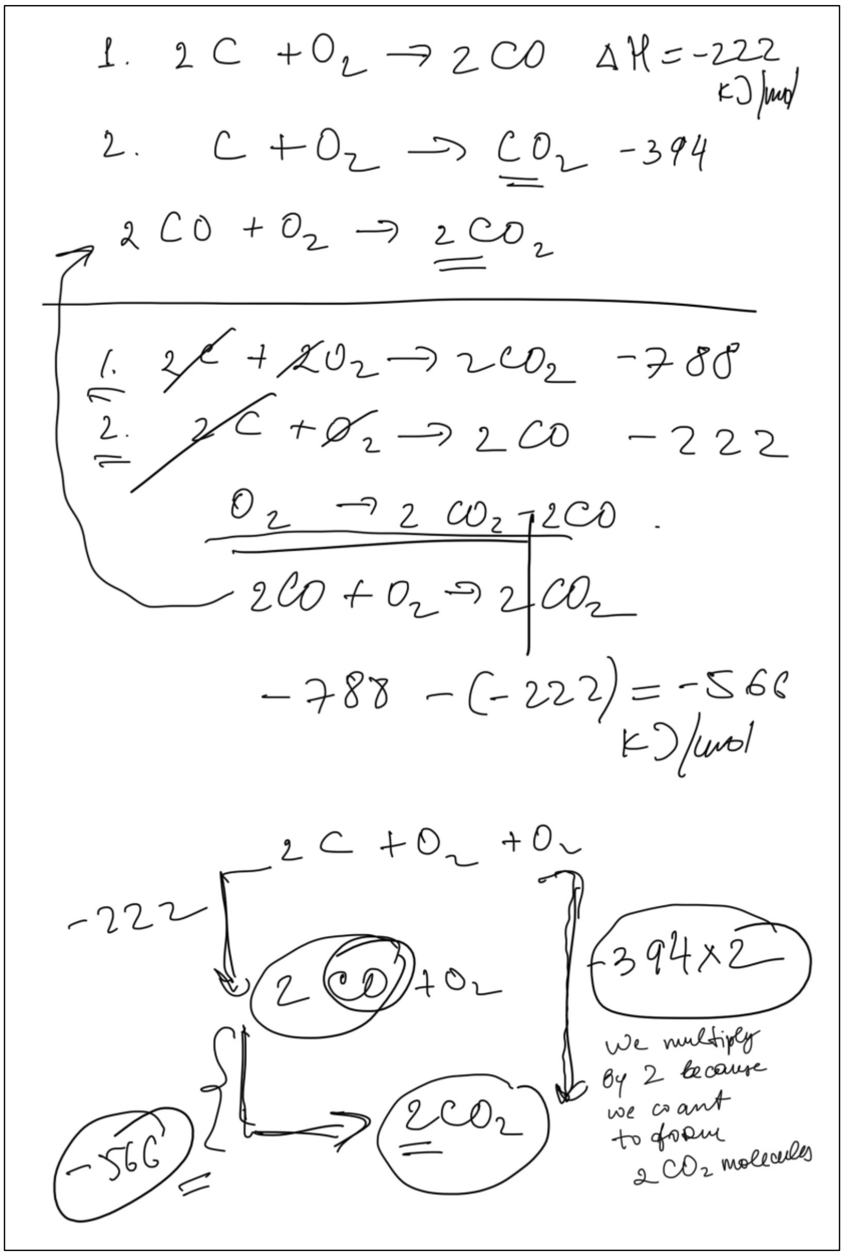
Let's look at the previous home work. Calculate enthalpy change for the following reaction

$2CO(g) + O_2(g) \rightarrow 2CO_2(g)$

The enthalpy change for these reactions are known

$2C(s) + O_2(g) \rightarrow 2CO(g)$ **Δ** H=- 222 kJ/mol

$C(s) + O_2(g) \rightarrow CO_2(g)$ **Δ** H=- 394 kJ/mol



Multiply reaction number 2 by 2, because we need to count 2 CO_2 in the final reaction.

Subtract reaction 2 from reaction1 including enthalpy changes, we will get our final reaction and the enthalpy change.

Calculate enthalpy change for the reaction **$Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$**
When you know standard enthalpy change of formation of the products and reactants.
The **enthalpy change of formation** (ΔH_f) refers to the heat energy change that occurs when **one mole** of a substance is formed from its constituent elements in their **standard states** under standard conditions (298 K, 1 atmosphere pressure). It is a type of **enthalpy change**, a thermodynamic quantity used to describe the energy change in chemical reactions.

$\Delta H_f^{\ominus}$ $Fe_2O_3 = -822$ kJ/mol

$\Delta H_f^{\ominus}$ $CO = -111$

$\Delta H_f^{\ominus}$ $CO_2 = -394$

$\Delta H_f^{\ominus}$ - standard enthalpy change of formation.

Element in its standard state has $\Delta H_f^{\ominus} = 0$

$\Delta H_f^{\ominus}$ for iron = 0

Knowing $\Delta H_f^{\ominus}$ for the above substances calculate enthalpy change for the following reaction: $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$.

1. $2Fe + \frac{3}{2} O_2 \rightarrow Fe_2O_3$ $\quad \Delta H = -822$

formation of Fe_2O_3

2. $C + \frac{1}{2} O_2 \rightarrow CO$ $\quad -111$

formation of CO

3. $C + O_2 \rightarrow CO_2$ $\quad -394$

formation of CO_2

ΔH_r = sum ΔH_f (products) − sum ΔH_f (reactants)

symbol for sum Σ

$\Delta H_r = \Sigma \Delta H_f (products) - \Sigma \Delta H_f (reactants)$

our products 2 Fe and 3 CO_2

$2 \times 0 + 3 \times (-394)$

our reactants Fe_2O_3 and 3 CO

$-822 + (3 \times -111)$

$\Delta H_r = 3 \times (-394) - (-822 + (3 \times -111)) =$

$= -27$ kJ/mol

Questions:

1. Calculate the enthalpy change for the reaction
   BrF (g) + $2F_2$ (g) → BrF_5 (l)
   We know that
   BrF (g)+ F_2 (g) → BrF_3 (l) (g) **Δ** H=- 242 kJ/mol
   BrF_3 (gl+ F_2 (g) → BrF_5(l) (g) **Δ** H=- 158 kJ/mol
2. Calculate the enthalpy change for the reaction
   ClF_3 (g) + F_2 (g) → ClF_5 (g)
   We know that
   Cl_2 (g) + $3F_2$ (g) → $2ClF_3$ (g) **Δ** H=- 328 kJ/mol
   Cl_2(g) + $5F_2$ (g) → $2ClF_5$ (g) **Δ** H=- 510 kJ/mol
3. Calculate the enthalpy change for the reaction
   $4NH_3$(g) + $5O_2$ (g) → 4NO (g) + $6H_2O$ (g)
   Standard enthalpy change of formation for NH_3(g) = -46 kJ/mol, for NO (g) = 90 kJ/mol, for H_2O (g) = -242 kJ/mol