Exercise 1 solution

1. (Exercise 1.7 from O'Hayre)

   Energy is released when hydrogen and oxygen react to produce water. This energy comes from the fact that the final hydrogen–oxygen bonds represent a lower total energy state than the original hydrogen–hydrogen and oxygen–oxygen bonds. Calculate how much energy (in kilojoules per mole of product) is released by the reaction

   $$H_2 + \tfrac{1}{2}O_2 \rightleftharpoons H_2O \tag{1.12}$$

   at constant pressure and given the following standard bond enthalpies. Standard bond enthalpies denote the enthalpy *absorbed* when bonds are *broken* at standard temperature and pressure (298 K and 1 atm).

Standard Bond Enthalpies
H–H = 432 kJ/mol
O = O = 494 kJ/mol
H–O = 460 kJ/mol

<u>Solution</u>

The reaction can be written also as

$$2H_2 + O_2 \rightarrow 2H_2O \quad \text{or} \quad \text{H–H + H–H + O=O} \rightarrow \text{H–O–H} \quad \text{H–O–H}$$

which is the original reaction multiplied by two for clarity. The overall heat of this reaction can be calculated as follows:

Bond	Bond energy (kJ/mol)	Number of broken bonds	Energy required (kJ/mol per reaction)	Number of bonds formed	Energy released (kJ/mol per reaction)
H–O	460	0	0	4	1840
H–H	432	2	864	0	0
O=O	494	1	494	0	0

Sum of energy required = 1358 kJ/mol

Sum of energy released = 1840 kJ/mol

Net difference = Sum of energy required - Sum of energy released = - 482 kJ/mol.

The negative sign means that energy is released in the reaction. To get the energy per mole of product (water) we need to divide by two which is the stoichiometric coefficient of H_2O molecules in the calculated reaction.

Answer: Net energy <u>released</u> per mole of H_2O = 482 kJ/mol / 2 = <u>**241 kJ/mol**</u>.

Note: It would have been equally OK to make the calculation for the original reaction, taking into account that that only a "half" oxygen molecule is consumed per produced H_2O.

2. Let's examine the electrolysis of water. The general reaction is given by:

$$2H_2O \rightarrow 2H_2 + O_2$$

   Is this an endothermic reaction (energy required) or exothermic reaction (energy released)? How much energy (kJ/mol) is absorbed or released per mole of H_2O consumed?

Solution

This reaction is the opposite of to the problem 1, and so, obviously equal amount of energy is required in it (per mole of consumed H_2O) than was released in reaction of problem 1. For the sake of practice, let's nevertheless do the corresponding calculation.

The overall heat of reaction can be calculated as follows:

Bond	Bond energy (kJ/mol)	Number of broken bonds	Energy required (kJ/mol per reaction)	Number of bonds formed	Energy released (kJ/mol per reaction)
H−O	460	4	1840	0	0
H−H	432	0	0	2	864
O=O	494	0	0	1	494

Sum of energy required = 1840 kJ/mol

Sum of energy released = 1358 kJ/mol

Net difference = Sum of energy required - Sum of energy released = 482 kJ/mol.

Because the sign of positive, energy is required.

The thermochemical equation is:

$2H_2O + 482\ kJ/mol \rightarrow 2H_2 + O_2 + 0\ kJ/mol$

3. Label the following reactions as oxidation or reduction reactions:

   Solution

   a) $Cu \rightarrow Cu^{2+} + 2e^-$ (Oxidation)
   b) $2H^+ + 2e^- \rightarrow H_2$ (Reduction)
   c) $O^{2-} \rightarrow ½O_2 + 2e^-$ (Oxidation)
   d) $CH_4 + 4O^{2-} \rightarrow CO_2 + 2H_2O + 8e^-$ (Oxidation)
   e) $O^{2-} + CO \rightarrow CO_2 + 2e^-$ (Oxidation)
   f) $½O_2 + H_2O + 2e^- \rightarrow 2(OH)^-$ (Reduction)
   g) $H_2 + 2(OH)^- \rightarrow 2H_2O + 2e^-$ (Oxidation)

4.

a) If a portable electronic device draws 1 A current at a voltage of 2.5V, what is the power requirement for the device?

b) You have designed a fuel cell that delivers 1 A at 0.5 V. How many of your fuel cells are required to supply the above portable electronic device with its necessary voltage and current requirements?

c) You would like the portable electronic device to have an operating lifetime of 100 h. Assuming 100% fuel utilization, what is the minimum amount of H_2 fuel (in grams) required?

d) If this H_2 fuel is stored as a compressed gas at 500 atm, what volume would it occupy (assume ideal gas, room temperature)? If it is stored as a metal hydride at 5wt % hydrogen, what volume would it occupy? (Assume the metal hydride has a density of 10 g/cm^3.)

Solution

a) Power requirement: $P = UI \rightarrow P = (1\ A)(2.5\ V) = 2.5\ W$.

b) Current of a single cell is sufficient so there is no need to connect cells in parallel. Voltage of a single cell on the other hand is not sufficient so $\frac{2.5\ V}{0.5\ V} = 5$ cells have to be connected in series.

c) Each cell consumes 1 A worth of hydrogen for 100 h. Each hydrogen molecule produces 2 electrons so the amount of consumed hydrogen is $n = \dot{n}t = \frac{5 \times I}{zF} t = \frac{5 \times 1 \frac{C}{s}}{2 * 96485 \frac{C}{mol}} \times 100 \times 3600\ s = 9.33\ mol$. The total amount of supplied hydrogen (100% fuel utilization) is $m = Mn = \left(2\ \frac{g}{mol}\right)(9.33\ mol) = 18.66\ g$

d) Compressed gas: $pV = nRT \rightarrow V = \frac{9.33\ mol \times 8.314 \frac{J}{K\ mol} \times 300\ K}{500 \times 1.013 \times 10^5\ Pa} \approx 465\ cm^3$

Metal hydride: $\rho_{hydride} = \frac{m_{hydride}}{V} = \frac{m_{H_2}}{0.05 \times V} \rightarrow V = \frac{18.66\ g}{0.05 \times 10 \frac{g}{cm^3}} = 37\ cm^3$