Answer all the questions below as fully as you can then check your answers

1. What is the difference between homolytic and heterolytic bond fission?

2. What is a free radical and explain how chlorine gas can form chlorine free radicals?

a. Write an equation to show the formation of chlorine free radicals from chlorine gas.

3. Dichloromethane can be made by the reaction of chloromethane and chlorine gas.

a. Name the type of mechanism involved in this reaction.
b. What is formed during the initiation step of this reaction?
c. Write an equation to show the initiation step.
d. The propagation step in a free radical substitution reaction involves two separate steps.

i. Write equations for the first and second propagation steps for the production of dichloromethane from chloromethane.

ii. Write an overall equation for the propagation step by combining your 2 equations from part i above.

e. What happens during the termination step of a free radical substitution reaction?

i. Write an equation or equations for a possible termination step in the production of dichloromethane from chloromethane.

4. Bromoethane can be prepared by a free radical substitution reaction involving ethane (C_2H_6) gas and bromine gas (Br_2).

a. What are the essential conditions needed to start this reaction?

b. Explain why sunlight will break the Br-Br bond to form free radicals but not the C-C or C-H bonds in ethane.

c. Write an equation for the initiation step.

d. Write equations for each of the two propagation steps.

i. For each of the two step in the propagation equations what is always consumed and what is always produced?

c. Write an overall equation for the propagation step of this reaction.

d. As well as bromoethane this reaction can also produce dibromoethane and tribromoethane as products. Explain why these products form.

i. If an excess of bromine is used in this reaction what will be the final product?

e. How could you adjust the reaction conditions to ensure that bromoethane is the main product of the reaction?

5. Methylbenzene ($C_6H_5CH_3$) can be converted into chloro(methylbenzene) in a free radical substitution reaction.

$$C_6H_5CH_3 + Cl_2 \longrightarrow C_6H_5CH_2Cl + HCl$$

a. What are the essential conditions for this reaction to take place?

b. Write an equation for the initiation step in this reaction.

c. Write equations for the two propagation steps and then write an overall equation for the propagation step.

d. Write at least one equation for a possible termination step.

Answers

1. What is the difference between homolytic and heterolytic bond fission?

   In homolytic bond cleavage the two atoms which share the two electrons in a covalent bond between them get back their own electron from the covalent bond when it breaks. This results in the formation of atoms/molecules with unpaired electrons, that is free radicals. In heterolytic bond cleavage one atom in the covalent bond takes both the electrons, this results in the formation of anions and cations.

2. What is a free radical and explain how chlorine gas can form chlorine free radicals?

   A free radical is a species (atom/molecule/ion) which contains an unpaired electron or electrons.

a. Write an equation to show the formation of chlorine free radicals from chlorine gas.

The covalent bond between the chlorine atoms breaks and the two electrons within the bond are shared equally between each chlorine atom. This results in the formation of 2 chlorine free radicals.

3. Dichloromethane can be made by the reaction of chloromethane and chlorine gas.

a. Name the type of mechanism involved in this reaction.

   Free radical substitution reaction

b. What is formed during the initiation step of this reaction?

   The initiation step forms free radicals. In this case we want to turn chloromethane into dichloromethane, so a chlorine will have to be added to chloromethane for this to happen. So we need to form chlorine free radicals during the initiation step.

c. Write an equation to show the initiation step.

$$Cl_2 \longrightarrow 2Cl\bullet$$

d. The propagation step in a free radical substitution reaction involves two separate steps.

i. Write equations for the first and second propagation steps for the production of dichloromethane from chloromethane.

equation 1 $\quad CH_3Cl + Cl\bullet \longrightarrow \bullet CH_2Cl + HCl$

equation 2 $\quad \bullet CH_2Cl + Cl_2 \longrightarrow CH_2Cl_2 + Cl\bullet$

Each of the equations in the propagation steps should have a molecule and a radical on each side of the equation to ensure the chain reaction proceeds smoothly.

ii. Write an overall equation for the propagation step by combining your 2 equations from part i above.

equation 1 $\quad CH_3Cl + Cl\bullet \longrightarrow \bullet CH_2Cl + HCl$

equation 2 $\quad \bullet CH_2Cl + Cl_2 \longrightarrow CH_2Cl_2 + Cl\bullet$

overall equation $\quad CH_3Cl + Cl_2 \longrightarrow CH_2Cl_2 + HCl$

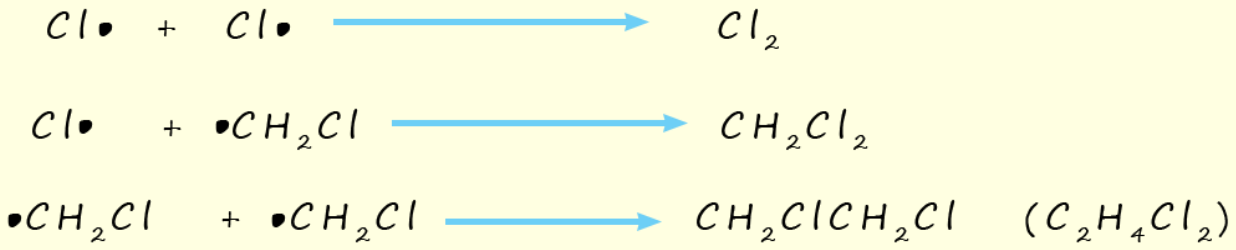
The overall equation is obtained by cancelling out the radicals as shown above.

e. What happens during the termination step of a free radical substitution reaction?

Two free radicals combine to form a stable molecule.

i. Write an equation or equations for a possible termination step in the production of dichloromethane from chloromethane.

To answer this find all the free radicals that are present in the reaction and simply combine them, each time two free radicals combine the chain reaction at this particular point ends!



4. Bromoethane can be prepared by a free radical substitution reaction involving ethane (C_2H_6) gas and bromine gas (Br_2).

a. What are the essential conditions needed to start this reaction?

Heat (anthing from around 150°C to 500°C) or UV light will break the Br-Br bond and cause the formation of free radicals, the initiation step.

b. Explain why sunlight will break the Br-Br bond to form free radicals but not the C-C or C-H bonds in ethane.

The Cl-Cl bond is weaker and there is not enough energy in the photon of UV light to break the stronger C-C and C-H bonds.

c. Write an equation for the initiation step.

d. Write equations for each of the two propagation steps.

equation 1 $CH_3CH_3 + Br\bullet \longrightarrow CH_3CH_2\bullet + HBr$

equation 2 $CH_3CH_2\bullet + Br_2 \longrightarrow CH_3CH_2Br + Br\bullet$

i. For each of the two step in the propagation equations what is always consumed and what is always produced?

Equations show that a radical reacts with a reactant molecule to produce a radical and a molecule of the product. It is important that if a free radical is consumed that another is produced to maintain the chain reaction.

c. Write an overall equation for the propagation step of this reaction.

The overall equation for the propagation steps is obtained by cancelling out all the free radicals from the reactants and products sides of the two equations as shown below:

equation 1 $CH_3CH_3 + Br\bullet \longrightarrow CH_3CH_2\bullet + HBr$

equation 2 $CH_3CH_2\bullet + Br_2 \longrightarrow CH_3CH_2Br + Br\bullet$

overall equation $CH_3CH_3 + Br_2 \longrightarrow CH_3CH_2Br + HBr$

d. As well as bromoethane this reaction can also produce dibromoethane and tribromoethane as products. Explain why these products form.

As the reaction proceeds the amount of the reactant ethane will decrease and the amount of product , bromoethane will increase. After a time the increasing concentration of bromoethane will means it will take over from the ethane as its concentration is falling.

i. If an excess of bromine is used in this reaction what will be the final product?

If a large excess of bromine is used then after each propagation step one of the hydrogen atoms in a molecule of ethene is replaced by a bromine atom. Ultimately all 6 hydrogen atoms on the ethene can be replaced by a bromine to form hexabromoethane.

e. How could you adjust the reaction conditions to ensure that bromoethane is the main product of the reaction?

Use a large excess of ethane gas in the reaction. This will help reduce the likelihood of more than hydrogen atom on ethane being replaced.

5. Methylbenzene ($C_6H_5CH_3$) can be converted into chloro(methylbenzene) in a free radical substitution reaction.

$$C_6H_5CH_3 + Cl_2 \longrightarrow C_6H_5CH_2Cl + HCl$$

a. What are the essential conditions for this reaction to take place?

Heat (anthing from around 150°C to 500°C) or UV light will break the Br-Br bond and cause the formation of free radicals, the initiation step.

b. Write an equation for the initiation step in this reaction.

$$Cl_2 \longrightarrow 2Cl\bullet$$

c. Write equations for the two propagation steps and then write an overall equation for the propagation step.

equation 1 $C_6H_5CH_3 + Cl\bullet \longrightarrow C_6H_5CH_2\bullet + HCl$

equation 2 $C_6H_5CH_2\bullet + Cl_2 \longrightarrow C_6H_5CH_2Cl + Cl\bullet$

d. Write at least one equation for a possible termination step.

Simply add together any of the free radicals present together to produce a stable molecule. This will terminate the chain reaction.