AS 91164 Demonstrate understanding of bonding, structure, properties and energy changes

Help Sheet for the Energy Calculations I

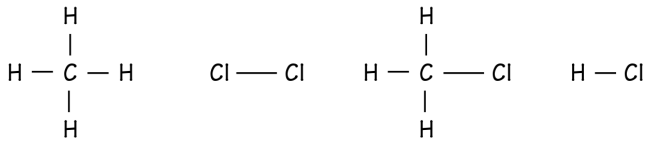
Questions involving bond enthalpies e.g. questions that look like.....

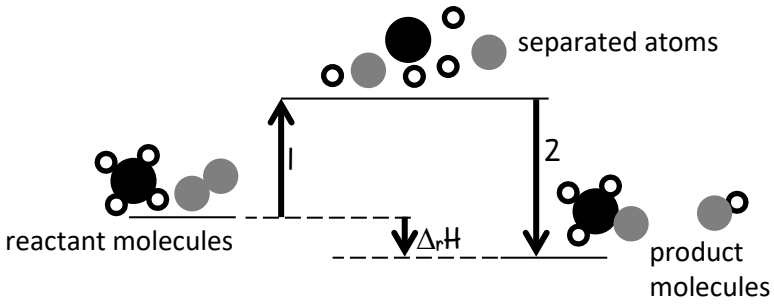
Chlorine reacts with methane to form chloromethane and hydrogen chloride, as shown in the equation below.

$$CH_4(g) + Cl_2(g) \rightarrow CH_3Cl(g) + HCl(g)$$

Use the bond enthalpies opposite to calculate Δ_rH^o for this reaction.

Consider the species involved in the reaction.





1. Bond breaking (endothermic)
2. Bond making (exothermic)

We are trying to find Δ_rH.

Average bond enthalpies have the units of kJ mol^{-1}.

They show the energy required to break 1 mol of a particular bond.

Bond	Bond enthalpy / kJ mol^{-1}
H-Cl	431
C-H	414
C-Cl	324
Cl-Cl	242

Average bond enthalpies are always listed as + numbers.

The value is + or - depending upon whether bonds are being broken (+) or formed (-).

To break bonds is endothermic; to make the same bonds is exothermic e.g if

$O=O \rightarrow O + O$ +498 kJ mol^{-1} then

$O + O \rightarrow O=O$ -498 kJ mol^{-1}

$\Delta_rH^o = \sum$(bonds broken) - $\sum$(bonds made)

where $\sum$ means "the sum of"

Before CH_4 and Cl_2 can react, 4 x C-H bonds and 1 x Cl-Cl bond have to be broken. Then 3 x C-H, 1 x C-Cl and 1 x H-Cl bonds need to be made/formed.

Bonds broken

- 4 x C-H 414 x 4
- Cl-Cl 242
- $\sum$(bonds broken) = 1656 + 242 = 1898

Bonds made/formed

- 3 x C-H 414 x 3
- C-Cl 324
- H-Cl 431
- $\sum$(bonds made) = 1242 + 324 + 431 = 1997

$$\Delta_rH^o = \sum(\text{bonds broken}) - \sum(\text{bonds made})$$

$$\Delta_rH^o = 1898 - 1997$$

$$\Delta_rH^o = -99.0 \text{ kJ mol}^{-1} \text{ (3 s.f.)}$$

Of course in this example opposite you could also choose to only look at the bonds that are changing in the reaction.

E.g.

- break 1 x C-H and 1 x Cl-Cl
- make 1 x C-Cl and 1 x H-Cl.

It would give you the same answer of $\Delta_rH^o = -99.0$ kJ mol^{-1}. Either method is fine.

2014: Hydrogen gas, $H_2(g)$, reacts with oxygen gas, $O_2(g)$, as shown by the following equation

$$H_2(g) + \tfrac{1}{2}O_2(g) \rightarrow H_2O(g) \quad \Delta_rH^o = -242 \text{ kJ mol}^{-1}$$

Given the average bond enthalpies in the table below, calculate the average bond enthalpy of the **O-H** bond in H_2O.

Bond	Average bond enthalpy / kJ mol^{-1}
H – H	436
O = O	498

Bonds broken are H-H and O=O

Bonds made are 2 x H-O (as H-O-H is made)

$$\Delta_rH^o = \sum\text{(bonds broken)} - \sum\text{(bonds made)}$$

$$-242 = 685 - 2x$$

$$2x = -927 \text{ kJ}$$

Don't forget the bonds formed are 2 x O-H in H_2O so divide by 2 to find O-H bond enthalpy. 927÷2 = 464 (3 s.f.)
So the average bond enthalpy of O-H bond is 464 kJ mol^{-1}.

Here is a harder one!!

The equation for the combustion of propan-1-ol is:

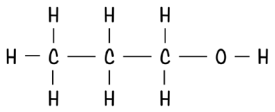
$$CH_3CH_2CH_2OH(g) + 4\tfrac{1}{2}O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g) \quad \Delta_rH = -2010 \text{ kJ mol}^{-1}$$

Calculate the bond enthalpy for the C=O bond, using the enthalpy of the reaction above and the bond enthalpy data in the table.

Bond	Bond enthalpy / kJ mol^{-1}
C–H	+414
C–O	+358
O=O	+498
C–C	+346
O–H	+463

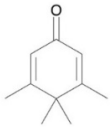
Strategy to solve

- Draw out $CH_3CH_2CH_2OH$ and work out the energy for all the bonds to be broken



- Calculate energy for bonds broken in 4.5 O_2 (4.5 x 498)
- **$\Delta_rH^o = \sum$(bonds broken) - $\sum$(bonds made)**
- Calculate energy for bonds made in $4H_2O$ (4 x H-O-H); this will be 8 x O-H bonds which will be 8 x 463 kJ
- We need to find energy for bonds made in $3CO_2$ (3 x O=C=O) , which is, of course, 6 x C=O bonds. Call this 6x.
- Find 6x and then divide by 6 to find x, the bond energy for one C=O bond.
- Answer is 826 kJ mol^{-1} (3 s.f.) (Written as + value like all average bond enthalpies).

Penguin



Penguinone