

Quadrant II – Transcript and Related Materials

Programme: Bachelor of Science (First Year)

Subject: Chemistry

Paper Code: CHC 102

Paper Title: Physical Chemistry and Organic Chemistry.

Unit: II

Module Name: Calculation of bond energy, bond dissociation energy and resonance energy from thermochemical data.

Module No: 05

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NOTES

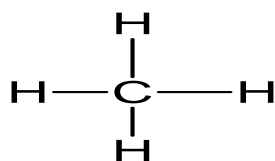
Bond energy

Bond energy is the average amount of energy required to dissociate one mole of bonds of that type present in the compound. Also called as enthalpy of formation of the bond. All chemical reactions involve breaking of old bonds followed by the making of new bonds.

- Bond breaking: ENDOTHERMIC \longrightarrow (C-H + ENERGY \longrightarrow C-H)
- Bond formation: EXOTHERMIC \longrightarrow (H + H \longrightarrow H-H + ENERGY)

For diatomic molecules, the bond energy is equal to the dissociation energy of the molecules. For polyatomic molecule (CH₄), the bond dissociation energies of the four C-H bonds are different. Hence, an average value is taken.

- Heat of reaction can be calculated from bond energy data.



$$\Delta H_{\text{reaction}} = \sum \text{Bond energies of reactants} - \sum \text{Bond energies of products}$$

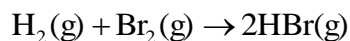
Bond	Enthalpy of formation (KJ/mol)	bond	Enthalpy of formation (KJ/mol)	Bond	Enthalpy of formation (KJ/mol)
H-H	435.1	C-Cl	330.5	C=O	711.3
H-F	564.8	C-Br	276.1	C-C	347.3
H-CL	430.9	C-S	259.4	C=C	615.0
H-Br	368.2	C=S	477.0	N=N	945.6
O-O	138.1	C-N	292.9	F-F	154.6
O=O	493.7	C=N	615.0	Cl-Cl	242.7
O-H	464.4	C°N	878.6	C°C	811.7
C-H	416.2	N-N	159.0	C-Fψ	439.3
C-O	351.4	N=N	418.4	Br-Br	192.5

FIG1. BOND ENERGIES

Problems on calculation of bond energy.

1. Calculate the enthalpy change for the reaction.

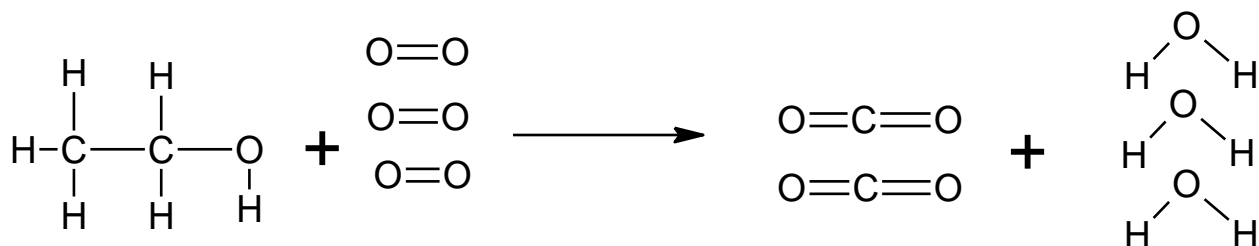
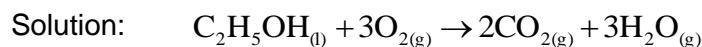
Given that the bond energies of H-H, Br-Br and H-Br are 435, 192 and 364 KJ mol⁻¹ respectively.



Solution: $\Delta H_{\text{reaction}} = \sum \text{Bond energies of reactants} - \sum \text{Bond energies of products}$

$$\begin{aligned} &= [\text{bond energy (H-H)} + \text{Bond energy (Br-Br)}] - [2 \times \text{Bond energy (H-Br)}] \\ &= [435 + 192] - [2 \times 364] \\ &= 627 - 728 = -101 \text{ KJ.} \end{aligned}$$

2. Calculate the enthalpy of combustion for ethanol using average bond energies.



$$\begin{aligned} \Sigma \text{bond energies (reactants)} &= (5 \times \text{C-H}) + (1 \times \text{C-O}) + (1 \times \text{O-H}) + (3 \times \text{O=O}) + (1 \times \text{C-C}) \\ &= (5 \times 413) + (1 \times 358) + (1 \times 467) + (3 \times 498) + (1 \times 347) \\ &= 4731 \text{ KJ/mol} \end{aligned}$$

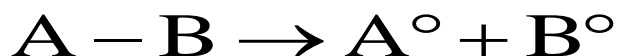
$$\begin{aligned} \Sigma \text{bond energies (products)} &= (4 \times \text{C=O}) + (6 \times \text{O-H}) \\ &= (4 \times 745) + (6 \times 467) \\ &= 5782 \text{ KJ/mol} \end{aligned}$$

$$\begin{aligned} \Delta H_{\text{REACTION}} &= \Sigma \text{bond energies (reactants)} - \Sigma \text{bond energies (products)} \\ &= 4731 - 5782 \\ &= -1051 \text{ KJ/mol} \end{aligned}$$

Bond dissociation energy

- It is also a measure of bond strength in a chemical bond.
- It is the change in enthalpy of a homolysis reaction at absolute zero (0 Kelvin)

where a molecule is broken down into two free radicals.



- It is not the same as average bond energy

DETERMINATION OF RESONANCE ENERGY

Generally, there is good agreement between the enthalpies of formation as calculated from bond energies and experimentally determined. If the compound exhibits resonance, there is a considerable difference between the two values. Difference between the two gives a measure of resonance energy.

- Assuming that benzene ring consists of 3 SINGLE BONDS (C-C), 3 DOUBLE BONDS (C=C) and 6 (C-H) BONDS. (KEKULE'S structure)
- Calculating dissociation energy:

$$\begin{aligned}\Delta H_d &= 3 (\Delta H_{C-C}) + 3 (\Delta H_{C=C}) + 6 (\Delta H_{C-H}) \\ &= 3 \times 347.3 + 3 \times 615 + 6 \times 416.2 \\ &= 5234.1 \text{ KJ mol}^{-1}\end{aligned}$$

Experimental value = 5535 KJ mol⁻¹. Actual energy required for dissociation of benzene is 151 KJ more than the calculated value. Thus the actual structure is more stable than the Kekule structure by 151 KJ (resonance energy)

The actual structure is now known to be resonance hybrid of two Kekule's structures.

