SUBJECT - CHEMISTRY
CLASS - B.Sc (Hons) PART-III
PAPER - V
TOPIC - Force Constant of a Chemical bond

Dr. Hari Mohan prasad Singh
Department of Chemistry
Dr. L.K.V.D College Tajpur Samastipur

Q What is force Constant of a chemical bond? How does it vary with (i) bond energy (ii) bond order and (iii) Stretching frequency?

Ans The vibrational frequency ($\bar{\nu}$) of a diatomic molecule is given by -

$$\bar{\nu} = \frac{1}{2\pi c}\sqrt{\frac{K}{\mu}} \quad \text{---} \quad (1)$$

where c = Velocity of light, K = force Constant and $\mu$ = reduced mass. From (1), we get -

$$\bar{\nu}^2 = \frac{1}{4\pi^2 c^2} \cdot \frac{K}{\mu}$$

or $K = 4\pi^2 c^2 \mu \bar{\nu}^2 \quad \text{---} \quad (2)$

$\Rightarrow K \propto \bar{\nu}$

we know that the restoring force (F) is proportional to the displacement (x) i.e

$F \propto -x$ [$\because$ F & x are acting in opposite directions]

or $F = -Kx \quad \therefore K = \frac{F}{x} = \frac{N}{m} = Nm^{-1}$

So the restoring force per unit displacement between bonded nuclei is called force constant. It is expressed in $Nm^{-1}$. If $\mu$ is the same as in case of hydrogen halides, the $\bar{\nu}$ will be proportional to K as per (2) -

$\mu_{HF} = \frac{1 \times 9}{20} = 0.95$ $\mu_{HBr} = \frac{1 \times 80}{81} = 0.99$

$\mu_{HCl} = \frac{1 \times 35}{36} = 0.97$; $\mu_{HI} = \frac{1 \times 27}{28} = 0.99$

for polyatomic molecules, the force constant is characteristic of the bond. The variance of bond energy (BE), bond order (BO) and stretching frequency ($\bar{\nu}$) with force constant (K) is shown as

| Bond | K-value | B.O | B.E | $\bar{\nu}$ |
|---|---|---|---|---|
| C – O | 490 ↓ increases | 1 | | |
| C = O | 1280 | 2 ↓ Inc | ↓ Inc | ↓ Inc |
| C ≡ O | 1880 ↓ | 3 ↓ | ↓ | ↓ |

The force constant (K) of a bond is determined spectroscopically with the help of IR spectrum of compounds where we get a graph of the percentage transmittance against wave number ($\bar{\nu}$). If $\bar{\nu}$ is known, K can be calculated using equation (2).

Q How is force constant related with IR frequency

Ans for poly atomic molecules, it assumed that each bond has a certain definite value of force constant which is characteristic of the bond and independent of the molecule in which it occurs. The force constant (K) of bonds increases with increase in bond order and decreases with increase in reduced mass e.g

| Bond | K-value | Bond | K-value | Bond | K-value |
|---|---|---|---|---|---|
| C – O | 490 | C – C | 460 | C – N | 480 |
| C = O | 1280 | C = C | 950 | C = N | 1210 |
| C ≡ O | 1880 | C ≡ C | 1580 | C ≡ N | 1750 |