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Study Notes on Molecular Spectroscopy

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Molecular Spectroscopy

In molecular spectroscopy, interaction of electromagnetic radiation with materials takes place. This interaction produces a spectrum which is helpful in determining structure or composition.
In this, either absorption or emission takes place as molecules undergo transition from one level to another. The mechanism involved is very complicated.
Mainly two primary interactions are involved in molecular spectroscopy and these are:

1. Force attraction (both repulsive and attractive) and Internal motion of nuclear framework
2. Interaction of nuclear magnetic and electrostatic moments

Let us discuss both points in detail.

Interaction can be divided into three categories as:

a. Electronic- Involves kinetic and potential energy
b. Vibrational- It arises due to motion of nuclei within the framework of molecule
c. Rotational- In the presence of a gas phase, molecule can undergo free rotation
d. Translational- If there is a change in centre of gravity, molecules possess translation energy.

Different types of spectroscopies are associated with different interactions and these are Visible, IR, UV, Raman, microwave, ESR, NMR, NQR

Basis for molecular spectroscopy:
It depends on the excitation of molecules and atoms by photons. Depending on the nature, molecules can excite either resonant vibration or electronic transitions. When a molecule undergoes vibrational transition, it appears in the IR region. Electronic transition takes place when a change in the electronic state of an atom/molecule is there and it appears in the UV-visible region.

Generally , molecular spectroscopy is referred to as absorption because it measures the energy loss.

Born -Oppenheimer approximation:

According to this approximation, the total energy of molecule is:

Total energy= Translational+vibrational+rotational+electronic

As translational energy is very small, so, it can be neglected, the above expression becomes:

Total energy= vibrational+rotational+electronic

Importance of molecular spectroscopy:

1. It is considered to be an important tool for identification and analysis of materials.
2. It has very much importance in various fields of detection.
3. It provides a precise method in finding constituents in material with unknown chemical composition.

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