ENGINEERING CHEMISTRY

Department of Science and Humanities

ENGINEERING CHEMISTRY

Module I- Molecular Spectroscopy

Class content:

- ***Born - Oppenheimer approximation***
- ***Energy level diagram of a diatomic molecule***

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Module I- Molecular Spectroscopy

Different types of energies possessed by a molecule

- **Translational energy** (E_{trans}): by virtue of translatory motion of the molecule
- **Rotational energy** (E_{rot}) : by virtue of rotation of a molecule about its centre of gravity
- **Vibrational energy** (E_{vib}): by virtue of periodic diaplacement of the atoms of a molecule about its equilibrium position
- **Electronic energy**(E_{elec}) : due to the different electronic arrangements in the molecule

Born-Oppenheimer approximation

- **Total energy** of a molecule is the sum of translational, rotational, vibrational and electronic energies, i.e.

$$E = E_{trans} + E_{rot} + E_{vib} + E_{elec}$$

- Translational energy is negligibly small. Hence Born-Oppenheimer approximation can be written as

$$E = E_{rot} + E_{vib} + E_{elec}$$

- Electronic, vibrational and rotational energies of a molecule are **completely independent** of each other
- Because the electronic energy levels are much farther apart than the vibrational energy levels which are again much farther apart than the rotational energy levels
- Can be written as

$$E_{rot} << E_{vib} << E_{elec}$$

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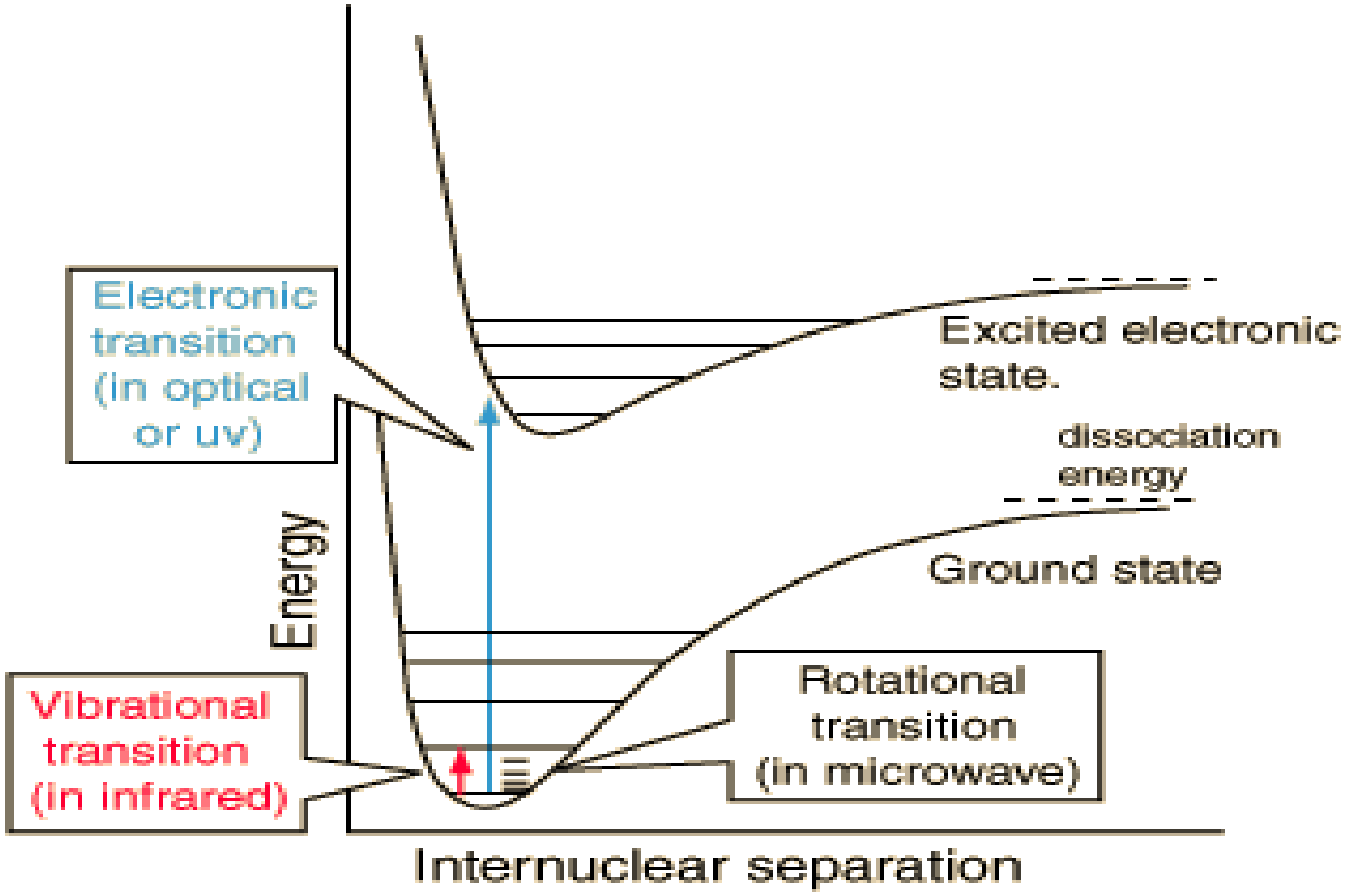
Molecular Spectroscopy

Energy level diagram for a diatomic molecule



Source:http://hyperphysics.phy-astr.gsu.edu/hbase/molecule/molec.html

THANK YOU

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