INTRODUCTION

Spectroscopy is the study of interaction of radiation with matter.

Vibrational Spectroscopy is useful for Understanding of

* **Molecular Motions**
* **Molecular Structure**
* **Physical & Chemical Properties**
* **Strength of Chemical Bonds etc.**

IR SPECTROSCOPY

Absorption of Light Energy

Applied for

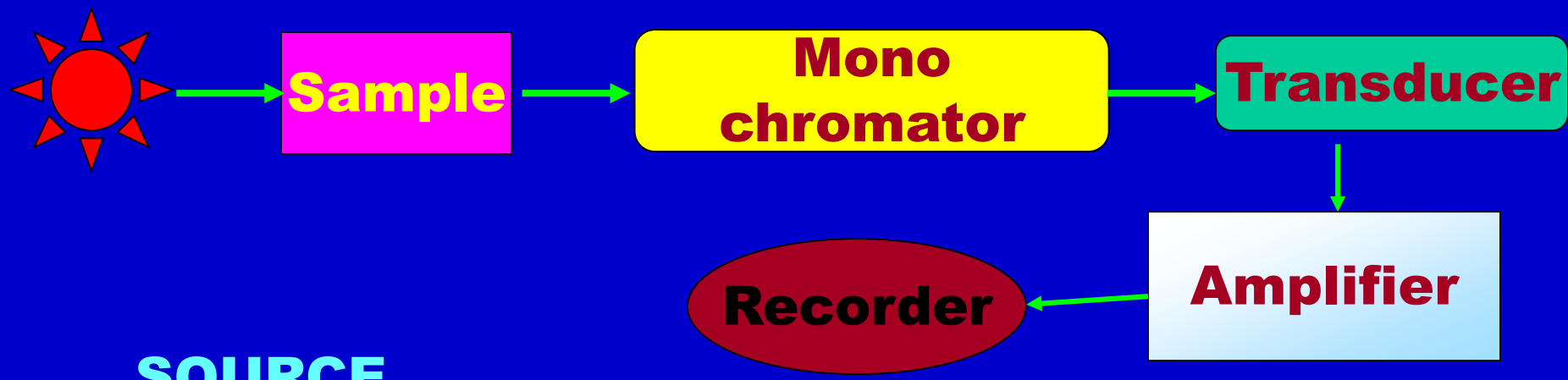
* **Identification of organic compounds**
* **Identification of functional groups**

Selection Rule

Change in dipole moment in a molecule is essential for IR active

Magnitude of the change in dipole moment decides the intensity of the IR Peaks

Units of IR Spectrometer



SOURCE

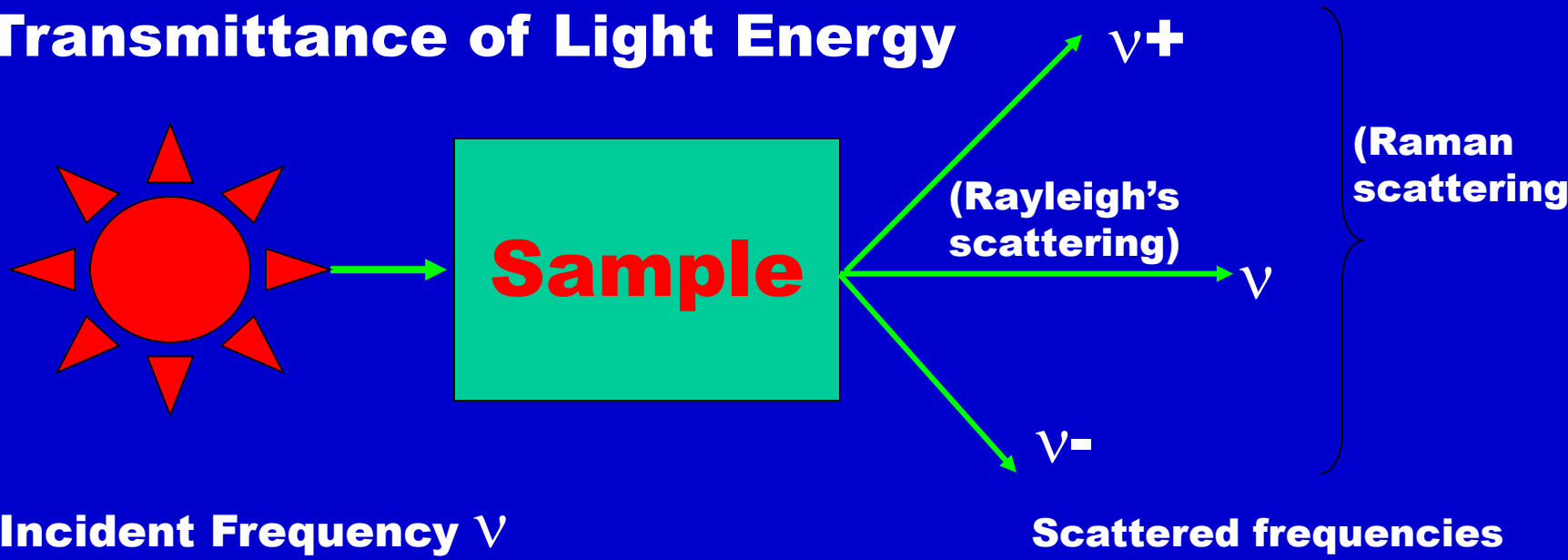
- Nd-YAG Laser operating at IR region
- Incandescent lamp
- Nernst Glower
- Globar Arc Lamps

SAMPLE HANDLING

- KBr pellets for recording Mid IR
- Polyethylene pellets for recording far IR

RAMAN SPECTROSCOPY

Transmittance of Light Energy



- ☺ **Argon Ion**
- ☺ **Krypton Ion**
- ☺ **Helium - Neon**
- ☺ **Diode Laser**
- ☺ **Nd : YAG**

Selection Rule

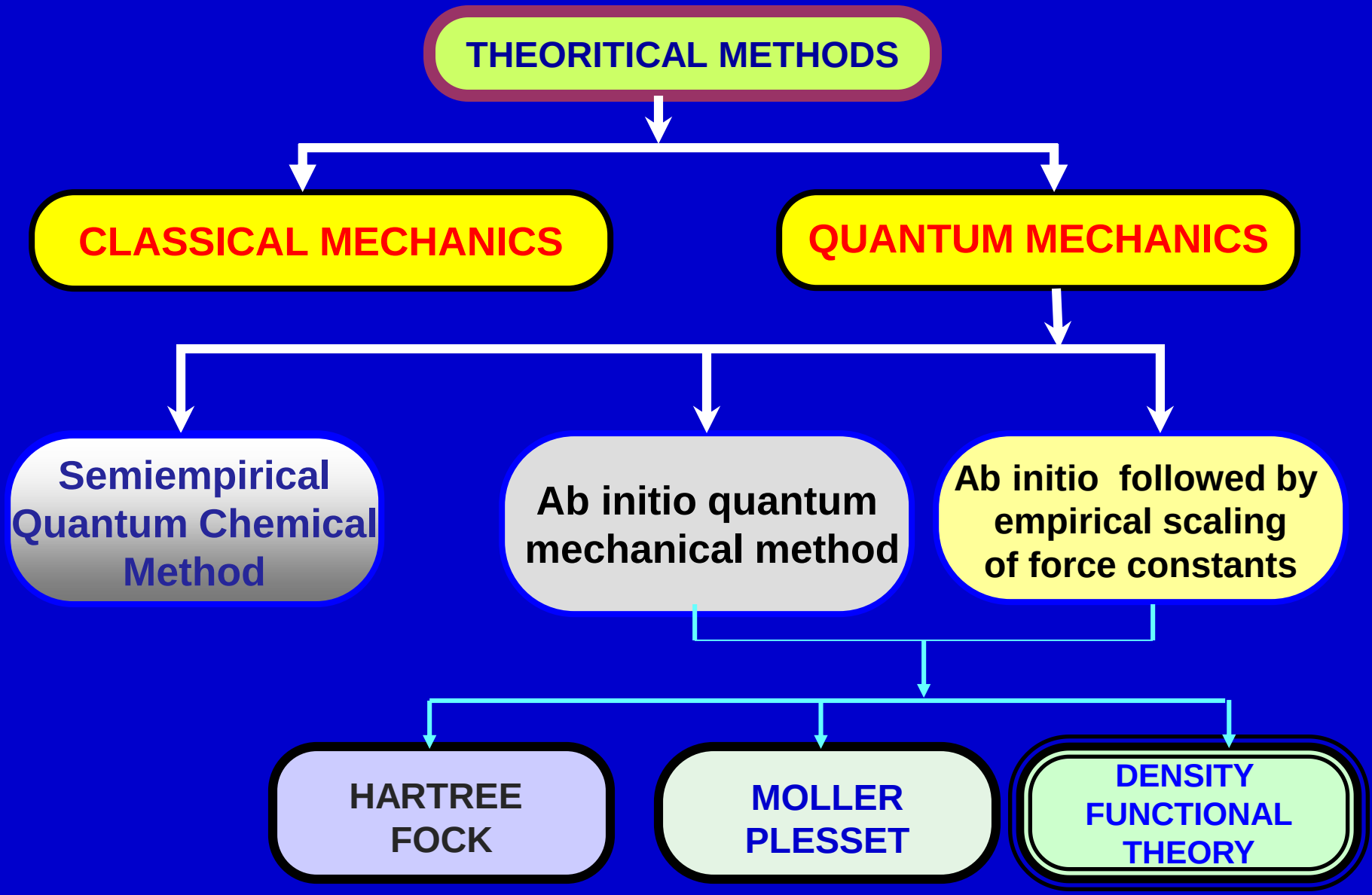
Change in polarizability

The stokes lines are more intense than antistokes lines

Introduction of laser is rebirth to Raman

It is a powerful analytical tool

- **Materials characterisation**
- **Identification of functional groups**
- **Crystal structure and symmetry etc.**


THEORITICAL METHODS
CLASSICAL MECHANICS
QUANTUM MECHANICS
Semiempirical Quantum Chemical Method
Ab initio quantum mechanical method
Ab initio followed by empirical scaling of force constants
HARTREE FOCK
MOLLER PLESSET
DENSITY FUNCTIONAL THEORY

Quantum Chemical Calculations

The assignment of bands in the vibrational spectra of polyatomic molecule is an essential step in applications of vibrational spectroscopy.

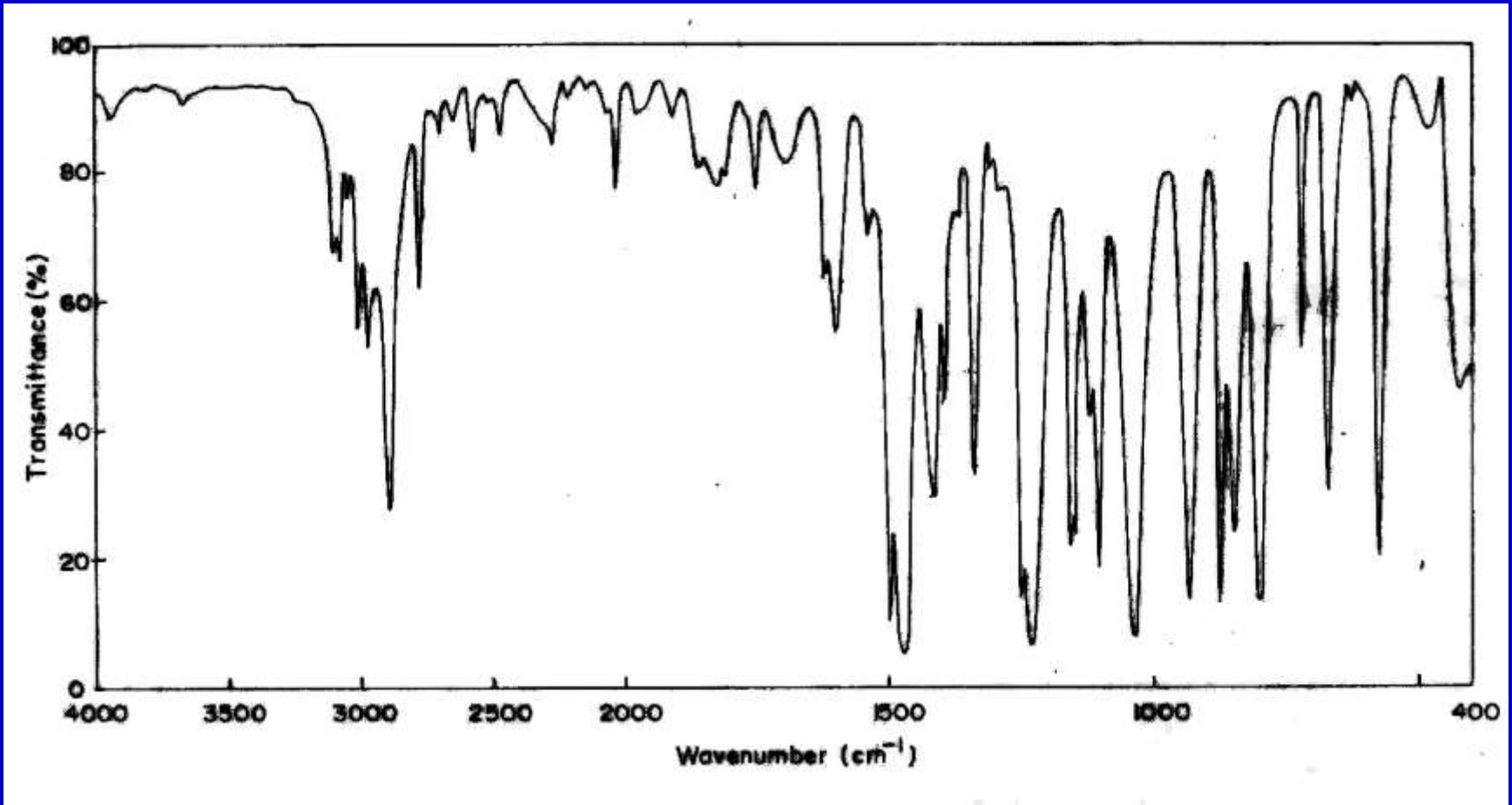
Now-a-days, with the development of sophisticated computational methods of theoretical chemistry, the vibrational frequencies and their intensities can be predicted theoretically and the vibrational spectra can also be simulated by applying QCM.

Density Functional Theory (DFT)

- Increasingly available and deliver force field of high accuracy
- In the frame work of DFT approach B3LYP [Becke's three parameter exchange function (B3) in combination with both the correlational functional of Lee, Yang and Parr (LYP)] combination is providing excellent result of Vibrational wave numbers
- B3LYP proved its ability in reproducing various molecular structure including vibrational spectra
- The combined use of DFT method, B3LYP functionals, Standard basis set yields good agreement between observed and calculated frequencies

INSTRUMENTATION

- **Instrumentation is an exciting and fascinating part of chemical analysis**
- **FTIR and FT Raman instrumentation techniques have been found to be useful in**
  - **identification of all types of organic and many types of inorganic compounds**
  - **determination of functional groups**
  - **determination of molecular composition of surfaces**
  - **determination of compounds in mixtures**



FTIR Spectrum

- The vibrational properties of the chosen compounds investigated by FTIR and FT-Raman spectroscopy reveal that they have more relevance to chemists and technologists.

- The chemistry behind the molecules plays a vital role in deciding the usefulness of the molecules.

- The vibrational assignments, TED and DFT calculations in this study may be useful for physicists & chemists for better understanding of vibrational behaviour of complex systems.

- The NLO properties possessed by the molecules have been revealed

- The FMOs play an important role in the electric and optical properties, as well as in UV–Vis spectra and chemical reactions.

A lower HOMO–LUMO energy gap explains the fact that eventual charge transfer interaction is taking place within the molecule.

- Furthermore, the polarizability, the first hyperpolarizability and total dipole moment of the chosen compounds have been calculated and the results are discussed