



**D.P. VIPRA COLLEGE**

**BILASPUR**

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WELL COME

# NUCLEAR QUADRUPOLE RESONANCE SPECTROSCOPY

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# INTRODUCTION:-

- ✘ NQR Spectroscopy was discovered by **H.G DUMLET** in 1951.
- ✘ Like NMR, NQR spectroscopy found in radiowave region of the electromagnetic radiation.
- ✘ The elongated have a prolate (assymmetric shape) spheriod symmetry and compressed one has an oblate shape.

# WHAT IS NQR?

- ✘ Nuclear quadrupole resonance or NQR is a technique related to nuclear magnetic resonance (NMR) which is used to detect atoms whose nuclei have a nuclear quadrupole moment.
- ✘ In NQR, on the other hand, nuclei with  $\text{spin} \geq 1$ , such as  $^{14}\text{N}$ ,  $^{35}\text{Cl}$  and  $^{63}\text{Cu}$ , also have an electric quadrupole moment so that their energies are split by an electric field gradient, created by the electronic bonds in the local environment .

# ELECTRIC QUADRUPOLE MOMENT(EQM)

- ✗  $eQ$  = Electric quadrupole moment, EQM
- ✗ If  $I > 1/2$ , Nucleus has EQM, EQM measures deviation of nuclear charge distribution from spherical symmetry
- ✗ **Some example of NQR;**

NUCLEUS	I	$q \times 10^{-28} \text{ m}^2$
$^2\text{H}$	1	$2.8 \times 10^{-3}$
$^{14}\text{N}$	1	$1.06 \times 10^{-3}$
$^{23}\text{Na}$	3/2	$9.7 \times 10^{-2}$
$^{35}\text{Cl}$	3/2	$-7.9 \times 10^{-2}$
$^{63}\text{Cu}$	3/2	-0.157
$^{93}\text{Nb}$	9/2	-0.2

# ***ELECTRIC FIELD GRADIENTS:-***

- ✘ Electric field gradients results from the non uniform distribution of electron density. These non uniform distribution is caused by
  1. **Non bonding electron(lone pair)**
  2. **Bonding electron**
- ✘ By properly selecting the axes components of EFG along x, y & z can be labelled as  $q_{xx}$ ,  $q_{yy}$ ,  $q_{zz}$



## NUCLEAR QUADRUPOLE RESONANCE APPLICATION:-

- ✘ The NQR frequencies for the various nuclei vary from several **kHz up to 1000 MHz** Their values depend on quadrupole moment of the nucleus, valent electrons state and type of chemical bond in which the studied atom participates.
- ✘ Using the NQR frequencies the quadrupole coupling constant(QCC) and asymmetry parameter ( $\eta$ ) can be calculated according to the different exact or approximate equations.
- ✘ For polyvalent atom NQR frequencies depend on coordination number and hybridization.

## USES OF NQR:-

- ✘ NQR has been used principally for investigating the electronic structure of molecules.
- ✘ Study of the structure of charge transfer complexes.
- ✘ Detection of crystal imperfection.
- ✘ Small imperfection destroy symmetry of internal electric field, lead to splitting or broadening of NQR.
- ✘ NQR offers the possibility of being applied to other tasks as well, including the non destructive evaluation of materials.

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**THANK YOU**