SYLLABUS

Practical aspects – Theory of I.R rotation vibration spectra of gaseous diatomic molecules – applications of I.R spectroscopy – Basic principles of F.T.I.R spectroscopy

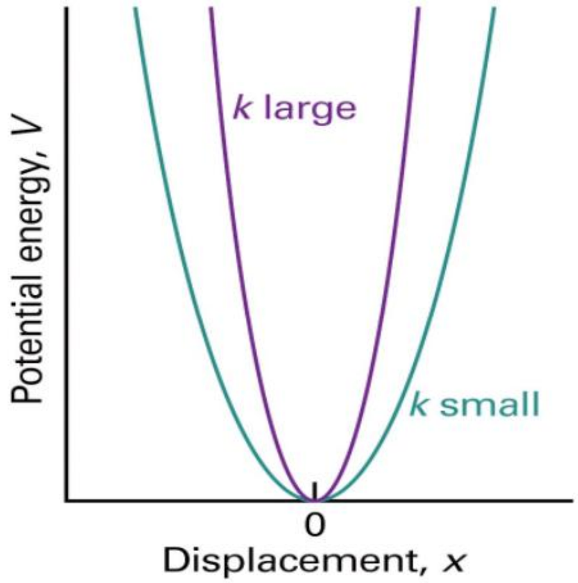
Classical and Quantum theory of Raman effect - Rotation vibration Raman spectra of diatomic and polyatomic molecules – Applications - Laser Raman spectroscopy

PRACTICAL ASPECTS:

We were discussing the sample holders, how we can take the sample in different containers and I had told you in the last class, that IR cells are constructed with sealed windows, which are separated by thin gaskets of copper and lead which are weighted with mercury; so, the whole assembly is securely clamped in a stainless still holder. As the mercury penetrates, a gasket it expands producing a tight seal. So, this is how we hold the sample. for films how do you take the infrared spectrum. So, for polymers, raisins and amorphous solids, the sample is usually dissolved in a volatile solvent and you evaporate the solvent, you will get a thin film of the material. So, a drop of the solution you can place it on the window and then seal the four edges as the solvent, evaporates a thin film of a homogeneous material is deposited which can be scan directly.

Theory of I.R rotation vibration spectra of gaseous diatomic molecules:

Molecular vibrations:



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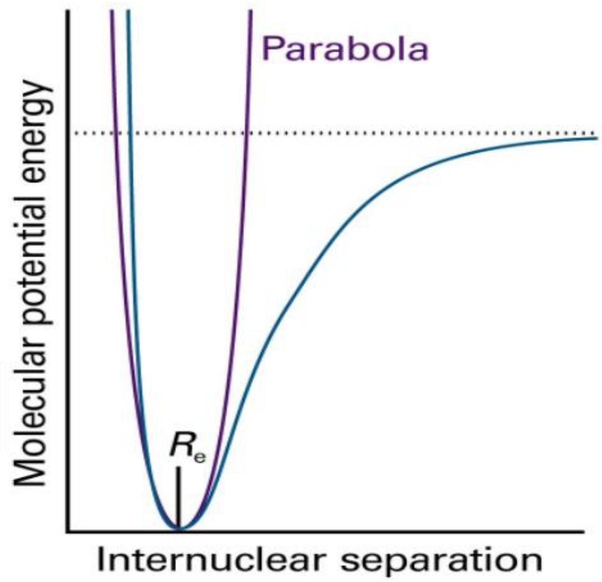

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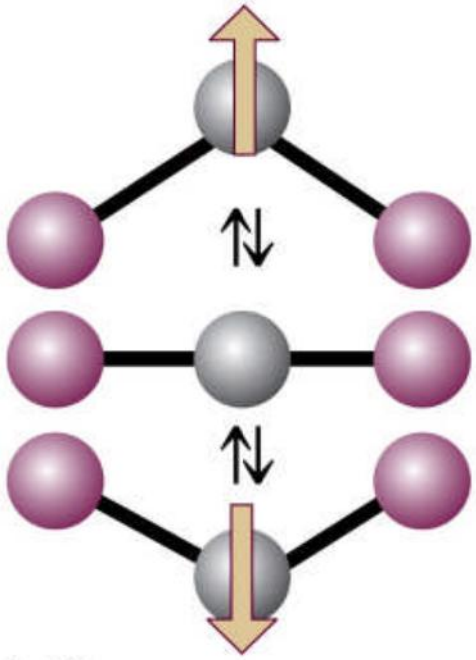
Typical potential energy curve of adiatomic molecule.Parabolic approximation close to Re.The steeper the walls of the potential, the stiffer the bond, the greater the force constant.

Selection rules:

Gross selection rule for a change invibrational state (absorption or emission):the electric dipole moment of the molecule(not necessarily permanent) must change when the atoms are displaced relative to one another.



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IR active molecules: heteronuclear diatomic.

IR inactive molecules: homonuclear diatomic. Not all the modes of polyatomic molecules are vibrationally active (e.g.: the symmetric stretch of CO2, in which the C –O–C bonds stretch and contract symmetrically is inactive.

Applications of I.R spectroscopy:

Infrared radiation lies between the visible and microwave portions of the electromagnetic spectrum.

Infrared waves have wavelengths longer than visible and shorter than microwaves, and have frequencies which are lower than visible and higher than microwaves.

TheInfrared region is divided into: near, mid and far-infrared.

Near-infrared refers to the part of the infrared spectrum that is closest to visible light and far-infrared refers to the part that is closer to the microwave region.

Mid-infrared is the region between these two.

The primary source of infrared radiation is thermal radiation. (heat)

It is the radiation produced by the motion of atoms and molecules in an object. The higher the temperature, the more the atoms and molecules move and the more infrared radiation they produce.

Any object radiates in the infrared. Even an ice cube, emits infrared.

Humans,atnormalbodytemperature,radiatemoststronglyintheinfrared,atawavelengthofabout10microns(Amicronisthetermcommonlyusedinastronomyforamicrometeroronemillionthofameter).Intheimagetotheleft,**theredareas**arethe**warmest**,followedby**yellow,greenandblue(coolest)**.

The bonds between atoms in the molecule stretch and bend, absorbing infrared energy and creating the infrared spectrum.

Raman spectroscopy:

Classical theory correctly predicts that Raman scattering should beweaker than Rayleigh scattering and that there is a simple linear dependence of Raman scattering on incident intensity and on sample concentration. With classical theory, Stokes/anti-Stokes intensity ratio. However, Boltzmann distribution will be major factor in determining relative Stokes and anti-Stokes intensity. The excited vibrational state will be only thermally populated, and Stokes intensity will be much larger than anti-Stokes. Full quantum mechanical treatment of Raman spectroscopy has been derived with time-dependent perturbation theory. Expressions for polarizability tensors involve sums over excited electronic states.

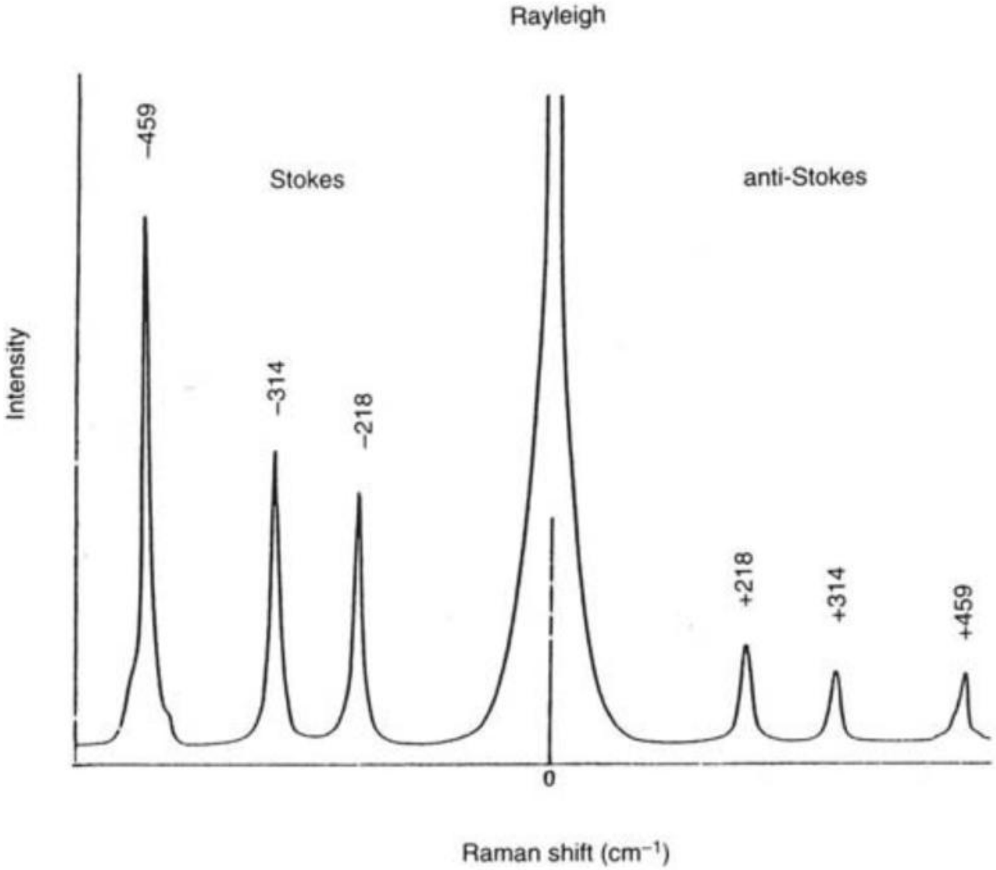
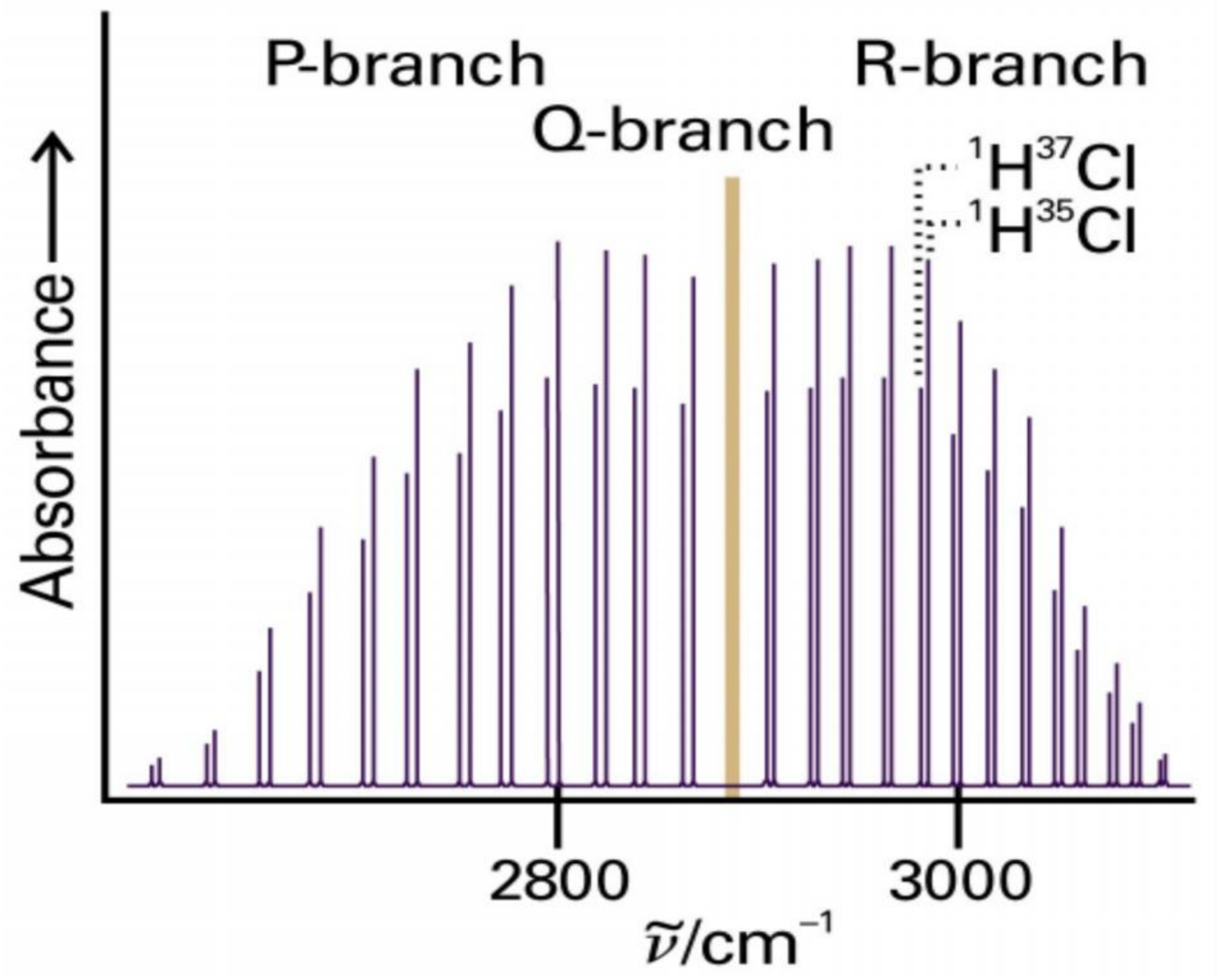


Figure 1-9 Raman spectrum of CCl_4 (488.0 nm excitation).

Rotation vibration Raman spectra of diatomic and polyatomic molecules:

Rotational change is expected since (classically) the transition leads to a sudden increase/decrease in instantaneous bond length. Therefore, rotation is retarded/accelerated by a vibrational transition.



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Detailed quantum mechanical analysis of simultaneous vibration and rotation changes shows that the rotational quantum number *J* changes by ±1 during the vibrational transition. If the molecule also possesses angular momentum bout its axis, then the selection rules.

POSSIBLE QUESTIONS

1. What is the basic principle of IR spectra?
2. Explain the construction and working of FTIR spectroscopy with suitable examples.
3. Explain the following with of Raman spectra.
    i) Rotation vibration spectra of diatomic molecules.
    ii) Any two applications
4. Explain the construction and working of Laser Raman Spectroscopy.
5. Explain the theory of IR rotation vibration spectra of gaseous diatomic molecules.
6. Explain the construction and working of Surface enhanced Raman scattering Spectroscopy.
7. Explain the theory of IR rotation vibration spectra of gaseous diatomic molecules.
8. What is Raman effect?
9. Explain the construction and working of Laser Raman Spectroscopy.
10. Explain the basic principles of IR spectroscopy and its applications.
11. Explain the concept of rotation vibration Raman spectra of diatomic molecules.
12. The Raman line associated with a vibrational mode which is both Raman and Infrared active is found at 4600 Å when excited by light of wavelength 4358 Å. Calculate the wavelength of the corresponding infrared band.

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DEPARTMENT OF PHYSICS
PHYSICS
SPECTROSCOPY (18PHP204)
MULTIPLE CHOICE QUESTIONS

QUESTIONS	**OPTION 1**	**OPTION 2**	**OPTION 3**	**OPTION 4**	**ANSWER**
In normal atomic spectra ------ changes its orbit by absorbing radiation					
Transition from a lower to upper level causes					
An atom can absorb -----	Valence electrons	electron in the inner orbit	nucleus	proton	Valence electrons
The principal qantum of the ground electronic state is	emission of radiation	absorption of radiation	scattering of radiation	none of the above	absorption of radiation
A photographic record of a spectrum is called	any amount of energy	only energy equal to the di	only energy less than th	only energy greater than the difference between two levels	only energy equal to the difference between two levels
The spectral lines of hydrogen atom where the transitions end at n = 2 level, form	0	1	-1	=+ or - 1	1
The study of both frequency and intensity of spectral lines is known as ----	spectrogram	spectrograph	spectrometer	spectroscope	spectrograph
For an energy level of principal quantum number n, the azimuthal quantum number can l	Lymann series	Bracket series	Pfund series	Balmer series	Balmer series
For principal quantum number n = 3, the values of azimuthal quantum number l are	spectroscopy	spectral study	spectrophotometry	spectrography	spectrophotometry
Hamiltonian of a system represents	n+1 values	n-1 values	n values	n^2 values	n values
For any real physical system represented by a Shrodinger wave equation, the eigen value	1,2,3,4	-3,-2,0,1,2,3	0,1,2	1,3,5,7	0,1,2
In the case of atomic spectra, the principal quantum numbers of two levels must be such	total energy of the system	only kinetic energy of the	only potential energy of	none of the above	total energy of the system
The splitting of spectral lines in the case of alkali metals was explained by considering	must be real and positive	can be complex but positiv	can be real but negative	can be anything	must be real and positive
For s orbital of electron the value of l is	they follow the selection rule	they follow the selection r	they follow the selectio	dn may be any positive integer	dn may be any positive integer
Zeeman effect is splitting of spectral lines in the presence of	orbital motion of the electror	spin of the electron	spin of the atom	spin of the nucleus	spin of the electron
The decoupling of nuclear spin angular momentum vector I and the total angular momen	0	1	2	3	0
For normal Zeeman effect, there are ----- lines when observed parallel to the magnetic fie	electric field	magnetic field	electric and magnetif fie	none of the above	magnetic field
The sodium D line is a member of -----	Pachen Back effect	Back-Goudsmit effect	Stark effect	Anomalous Zeeman effect	Pachen Back effect
Anomalous Zeeman effect occurs in atoms whose S is	2	3	5	A large number of lines	2
In normal zeeman effect, pi lines are -----	the principal siries	the diffuse series	the sharp series	the fundamental series	the principal siries
Which of the spectral series of hydrogen atom does not show fine structure?	greater than 1/2	equal to zero	less than zero	greater than zero	greater than zero
Anomalous Zeeman effect occurs in the presense of a	polarized in the direction of t	polarized perpendicular to	circularly polarized	non-polarized	polarized in the direction of the applied field
Hyperfine structure in atomic spectra is observed due to	Balmer series	Bracket series	Pfund series	Lymann series	Lymann series
The intensity of a spectral line mainly depends on	strong magnetic field	electric field	weak magnetic field	both electric and magnetic field	weak magnetic field
Hyperfine structure of rotational lines are due to	spin of the electron	spin of the nucleus	presence of isotope	temperature	spin of the nucleus
The molecule with permanent electric or magnetic dipole moment absorb	number of electron in the ato	the atomic number of the	the atomic mass of the	the number of atoms in the initial energy level	the number of atoms in the initial energy level
Stark modulation spectrometer is used to study	nuclear quadrupole moment	rotaion of the molecule	rotation of the atom	dipole moment	nuclear quadrupole moment
In normal zeeman effect, there are ------ lines when observeed perpendicular to the magr	infrared radiation	microwave radiation	UV radiation	radio waves	microwave radiation
The decoupling of L and S vectors due to the application of very high magnetic field is cal	IR spectrum	microwave spectrum	Raman spectrum	Fluorescence	microwave spectrum
The frequency of radiation absorbed due to rotational motion of molecules fall in the ----	2	3	4	0	3
The product eQq is known as	Pachen Back effect	Stern Gerlach effect	Stark effect	Back-Goudsmith effect	Pachen Back effect
The quantity eQ is known as the ----- of the nucleus	IR	UV	X-ray	Microwave	Microwave
The nuclear magneton (mu)N is ----- times the Bohr magneton (mu)B	electric dipole moment	magnetic dipole moment	Quadrupole coupling co	total magnetic moment	Quadrupole coupling constant
The angular momentum associated with the orbital quantum number L is given by	quadrupole moment	electric dipole moment	electric field strength	Magnetic field strength	quadrupole moment
The microwave region of the electromagnetic spectrum is between -----	1836	1/1836	2	none of the above	1/1836
The criterion for absorption of microwave is that the molecule should possess	L	L(L+1)	L(L+1)*h/(2pi)	[L(L+1)h/(2pi)}^1/2	[L(L+1)h/(2pi)}^1/2
For an asymmetric top molecule the moments of inertia are related as	1 mm and 300 mm	1mm and 30 mm	400 cm and 1200 cm	300 mm to 900 mm	1mm and 30 mm
In the case of a diatomic rigid rotator, the separation between nearby rotational lines is	either a permanent electric o	a permanent electric dipol	a permanent magnetic	none of the above	either a permanent electric or magnetic dipole moment
If the first line in a microwave absorption spectrum of a diaomic (rigid) rotator is observe	Ia = Ib = Ic	Ia = Ib not equal to Ic	Ia not equal to Ib = Ic	Ia not equal to Ib not equal to Ib	Ia not equal to Ib not equal to Ib
In the case of a diatomic rigid rotator, the energy difference between ground level and fir	B	3B	2B	4B	2B
In the case of non-rigid diatomic rotator, the separation between adjacent spectral lines	4B	6B	8B	10B	8B
In the case of non-rigid diatomic rotator, the reason for the separation between adjacent	2B	4B	6B	8B	6B
The vibrational excitation during rotation causes	increases with increasing J	decreasing with increasing	remains the same	can be either increasing or decreasing	decreasing with increasing J
The molecular system where the moments of inertia are related as Ia not equal to Ib not	increasing bond length during	due to reduction in speed	due to decreasing bond	none of the above	increasing bond length during rotation due to centrifugal force
Nuclei with spin quantum number I ------ lack spherical symmetry	increasing in B	reduction of B	no change	can either increase or decrease B	reduction of B
Pachen Back effect takes place in the presence of ----	symmetric top	asymmetric top	linear	spherical top	asymmetric top
When an atom with spin > placed in a weak magentic field, the spectral lines are split intc	> 1	> 0	= 1	> 1/2	> 1/2
A prolate symmetric top molecule has the relation between their moments of inertia as	very high electric field	very high magnetic field	weak electric field	weak magnetic field	very high magnetic field
When an atom of Carbon dioxide which does not possess a permanent dipole moment ar	Pachen Back effect	Back-Goudsmit effect	Anomalous zeeman effe	normal zeeman effect	Anomalous zeeman effect
A molecule whose moments of inertia are related as Ia = Ib > Ic is called	Ia < Ib = Ic	Ia = Ib < Ic	Ia > Ib = Ic	Ia = Ib > Ic	Ia < Ib = Ic
Rotation about the bond axis of a hetero nuclear diatomic molecule	it shows rotational spectrum	it does not show rotationa	it may or may not show	none of the above	it does not show rotational spectrum
The quantity which measures the deviation in the charge distribution in the nucleus from	oblate symmetric top	prolate symmetric top	oblate asymmetric top	none of the above	prolate symmetric top
The magnitude of the asymmetrical electric field surrounding the nucleus, due to electro	gives rotation spectrum	gives no rotation spectrum	gives some weak lines	none of the above	gives no rotation spectrum
The charge distribution in a nucleus with spin = 1/2 is	electric dipole moment	magnetic dipole moment	nuclear quadrupole mo	none of the above	nuclear quadrupole moment
When an atom with total angular momentum J is placed in a magnetic field, the magnetic	electric field gradient	magnetic field gradient	electric quadrupole mo	nuclear quadrupole moment	electric field gradient
The rotational selection rule is	non-spherical	prolate	oblate	spherical	non-spherical
Out of the three types of energy of a molecule, the lowest energy is due to ----	2J+1	J	J+1	J-1	2J+1
The total angular momentum of an atom is a vector sum of the ----	dJ = + or - 1	dJ = 0, +1 or -1	dJ = 0	dJ = 0, +1, -1, +2, -2,.....	dJ = + or - 1
Which of the following statements is not correct?	vibration of the molecule	electronic transition of the	rotation of the molecule	none of the above	rotation of the molecule
When the applied magnetic field is increased, the frequency of precession of the J vector	orbital angular momentum of	orbital angular momentum	orbital angular moment	spin angular momentum of the electron and the spin angula	orbital angular momentum of the electron, spin angular momentum of the electron and the spin angular momentum of the nucleus
	The robital angular momentu	S precesses around L	J and the nuclear spin a	F precesses around I	F precesses around I
	increases	decreases	remains the same	increases and then decreases	increases

SYLLABUS

Practical aspects – Theory of I.R rotation vibration spectra of gaseous diatomic molecules – applications of I.R spectroscopy – Basic principles of F.T.I.R spectroscopy

Classical and Quantum theory of Raman effect - Rotation vibration Raman spectra of diatomic and polyatomic molecules – Applications - Laser Raman spectroscopy

PRACTICAL ASPECTS:

We were discussing the sample holders, how we can take the sample in different containers and I had told you in the last class, that IR cells are constructed with sealed windows, which are separated by thin gaskets of copper and lead which are weighted with mercury; so, the whole assembly is securely clamped in a stainless still holder. As the mercury penetrates, a gasket it expands producing a tight seal. So, this is how we hold the sample. for films how do you take the infrared spectrum. So, for polymers, raisins and amorphous solids, the sample is usually dissolved in a volatile solvent and you evaporate the solvent, you will get a thin film of the material. So, a drop of the solution you can place it on the window and then seal the four edges as the solvent, evaporates a thin film of a homogeneous material is deposited which can be scan directly.

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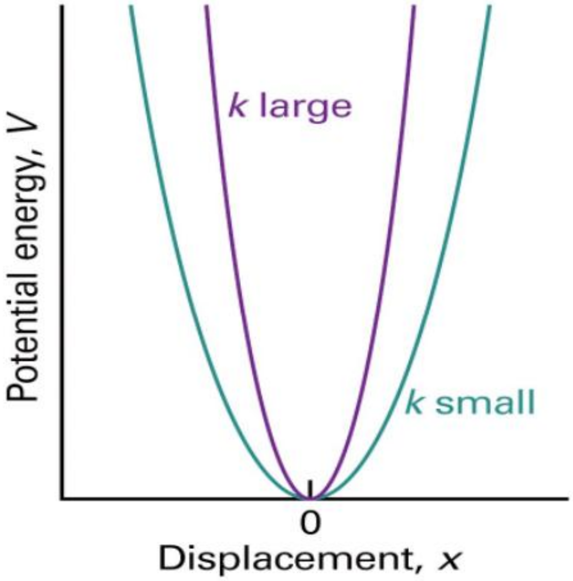
Molecular vibrations:



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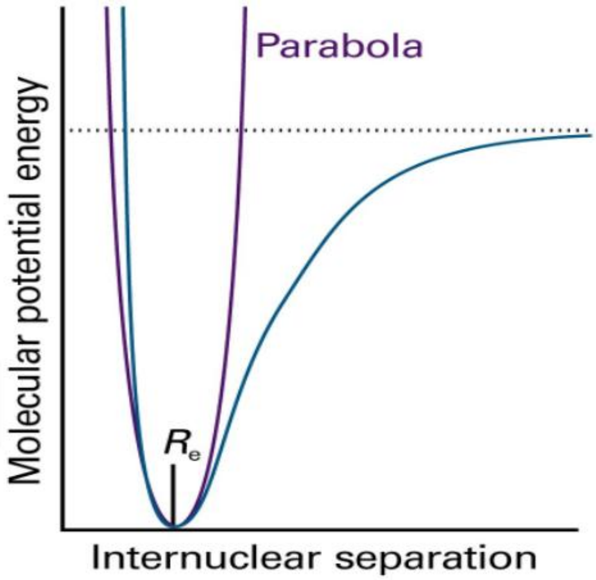

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Typical potential energy curve of adiatomic molecule.Parabolic approximation close to Re.The steeper the walls of the potential, the stiffer the bond, the greater the force constant.

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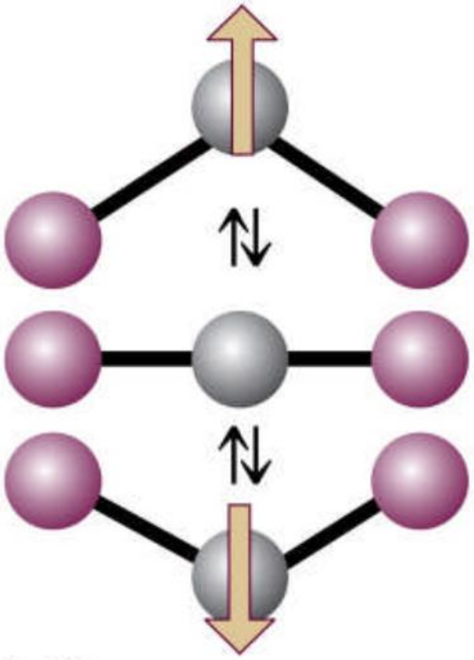

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IR active molecules: heteronuclear diatomic.

IR inactive molecules: homonuclear diatomic. Not all the modes of polyatomic molecules are vibrationally active (e.g.: the symmetric stretch of CO2, in which the C –O–C bonds stretch and contract symmetrically is inactive.

Applications of I.R spectroscopy:

Infrared radiation lies between the visible and microwave portions of the electromagnetic spectrum.

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TheInfrared region is divided into: near, mid and far-infrared.

Near-infrared refers to the part of the infrared spectrum that is closest to visible light and far-infrared refers to the part that is closer to the microwave region.

Mid-infrared is the region between these two.

The primary source of infrared radiation is thermal radiation. (heat)

It is the radiation produced by the motion of atoms and molecules in an object. The higher the temperature, the more the atoms and molecules move and the more infrared radiation they produce.

Any object radiates in the infrared. Even an ice cube, emits infrared.

Humans,atnormalbodytemperature,radiatemoststronglyintheinfrared,atawavelengthofabout10microns(Amicronisthetermcommonlyusedinastronomyforamicrometeroronemillionthofameter).Intheimagetotheleft,**theredareas**arethe**warmest**,followedby**yellow,greenandblue(coolest)**.

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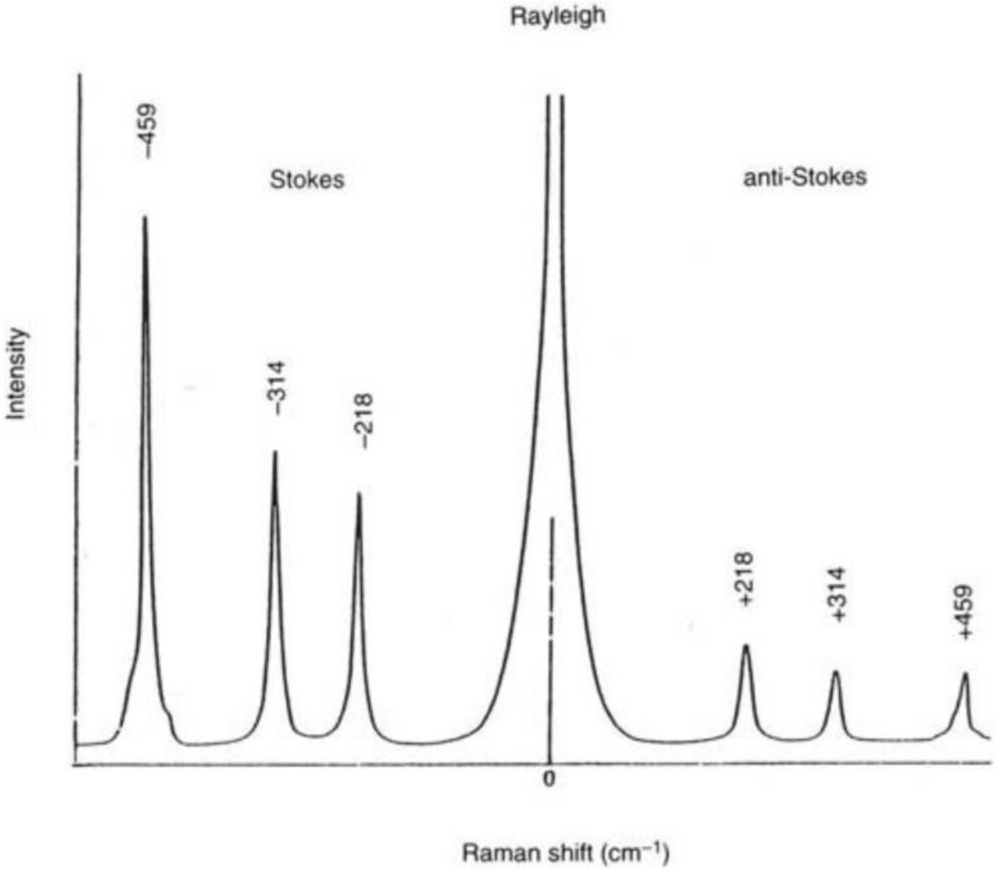

Figure 1-9 Raman spectrum of CCl_4 (488.0 nm excitation).

Rotation vibration Raman spectra of diatomic and polyatomic molecules:

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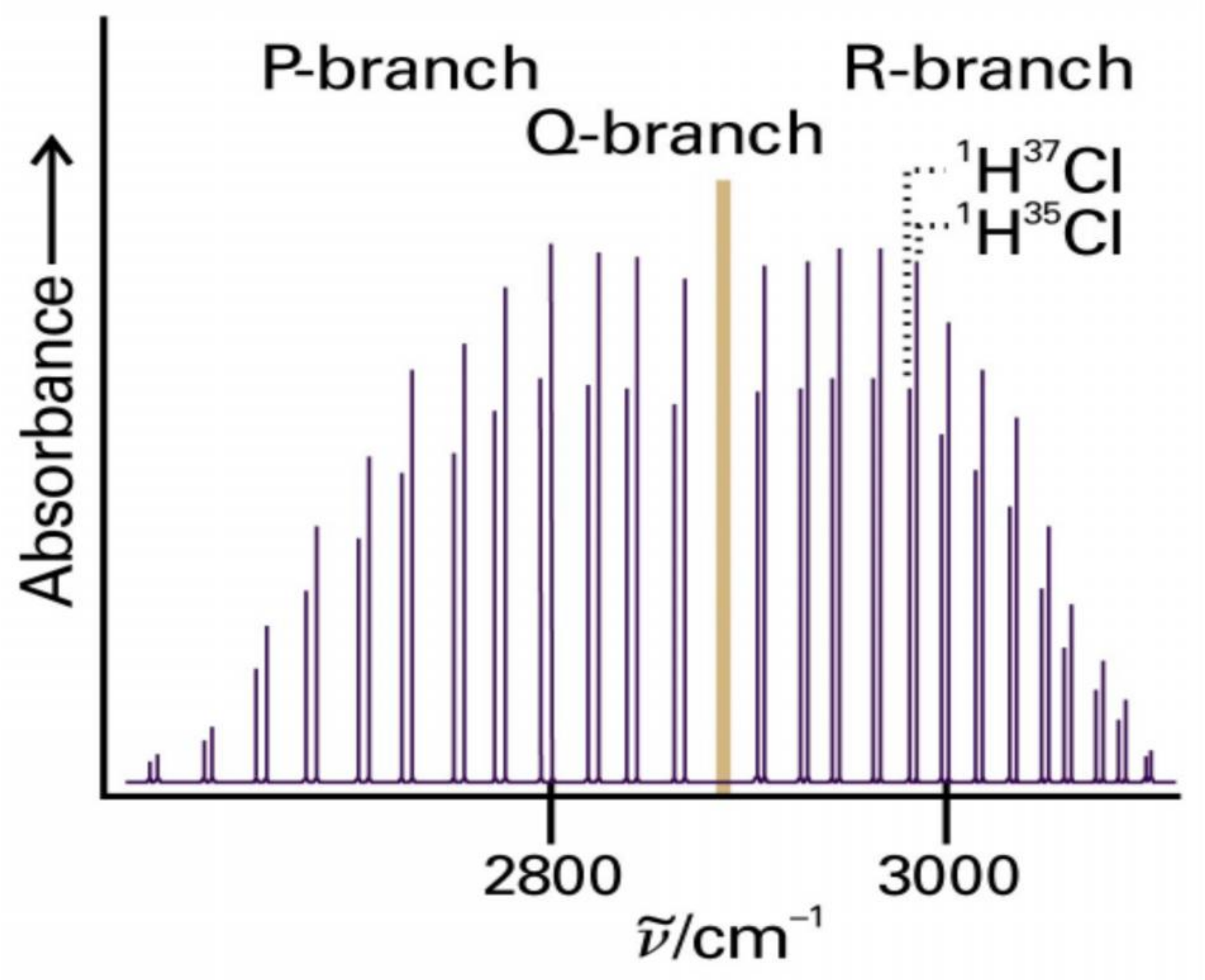

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Detailed quantum mechanical analysis of simultaneous vibration and rotation changes shows that the rotational quantum number *J* changes by ±1 during the vibrational transition. If the molecule also possesses angular momentum bout its axis, then the selection rules.

POSSIBLE QUESTIONS

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SPECTROSCOPY (18PHP204)
MULTIPLE CHOICE QUESTIONS

QUESTIONS
UNIT - II

Change in electric dipole moment during vibration gives rise to absorption in	**OPTION 1**	**OPTION 2**	**OPTION 3**	**OPTION 4**	**OPTION 5**	**OPTION 6**	**ANSWER**
Water molecule has ---- number of modes of vibraiton							
Raman scattering occurs due to ---- of molecule	visible spectrum	NMR spectrum	IR spectrum	microwave spectrum			IR spectrum
Glass is unsuitable as a lens for IR studies due to its ----	9	4	3	5			3
Mutual exclusion principle of Raman and IR spectra is applicable for	change in dipole moment	change in polarizability	change in magnetic dipol	change in quadrupole oment			change in polarizability
Which of the following spectra is independent of the exciting frequency	hardness	transmittence	dispersion	absorption			absorption
Hot bands are IR absorption involving vibrational levels ----	symmetric top molecules	asymmetric top molecules	molecules with centre of	diatomic molecules			molecules with centre of symmetry
Unlike in the case of other branches of spectroscopy, Raman spectroscopy is a ---- process	Raman	IR	Microwave	Electronic spectra			Raman
For a linear molecule the relation between the moments of intertia is	v =0 to v = 1	v = 0 to v = 2	v = 1 to higher values of	v = 1 to v = 2 only			v = 1 to higher values of v
The lines with frequency more than that of the exciting line in Raman spectra are called	scattering	absorption	emission	Fluorescence			scattering
Virtual energy level concept is used to explain	Ia=Ib=Ic	Ia=0, Ib=Ic not equal to 0	Ia < Ib < Ic	Ia > Ib > Ic			Ia=0, Ib=Ic not equal to 0
When the virtual energy levels coincide with actual enregy level it is called	Stokes lines	Rayleigh lines	antistokes lines	compton lines			antistokes lines
IR spectroscopy involves	IR absorption	Raman scattering	microwave absorption	none of the above			Raman scattering
Out of the three types of energies of a molecule, rotational, vibrational and electronic, the lo	resonance raman scattering	inverse raman scattering	surface enhanced raman	none of the above			resonance raman scattering
The most accurate method of determination of inter-nuclear distance, and bond angles in m	absorption	emission	scattering	stimulated emision			absorption
Pure rotational raman lines can be observed only in	electronic	rotational	vibrational	vibrational-rotational			electronic
In IR spectra, the first overtone lines are due to transition from	IR	Raman	Microwave	UV			IR
In the case of rotational raman spectra the selection rule dJ = 0 refers to	heavy molecules	light polyatomic molecules	heavy polyatomic molecu	light diatomic molecules			light diatomic molecules
IR and Raman spectroscopy are said to be ----- to each other	v=0 to v=2	v=1 to v=2	v=0 to v=1	v=0 to v=3			v=0 to v=2
Raman spectroscopy is due to -----	antistokes lines	stokes lines	both a and b	Rayleigh lines			Rayleigh lines
Which of the following statements is not true?	complementary	opposite	repetition	inverse			complementary
Classical theoretical expalnation of Raman effect could not explain	change in dipole moment	change in polarizability	change in magnetic dipol	none of the above			change in polarizability
Polarizability tensor has ----- components	Raman scattering cannot be ex	Microwave spectroscopy is	IR spectroscopy is an abs	Raman scattering is a scattering process			Raman scattering cannot be excited by any frequency
Even though polarizability is a tensor of nine components, there are only ----- independent c	rotational raman lines	vibrational raman lines	rotation-vibration structu	intensity of stokes and antistokes lines			intensity of stokes and antistokes lines
In the case of anti Stokes Raman scattering	7	3	9	5			9
Zero point energy is the energy possessed by the molecule when it is in the	6	8	3	7			6
Nernst Glower is normally used as a source of	energy is absorbed by the mole	energy is given by the mole	both photon and molecu	no energy transfer			energy is given by the molecule to the photon
The number of vibrational modes for a linear molecule is	lowest vibrational level	lowest rotational level	lowest electronic level	none of the above			lowest vibrational level
A grating is uses the phenomenon of ----- to split the spectral lines into different frequencies	Microwave radiation	IR radiation	Raman spectrum	UV spectrum			IR radiation
Rocksalt prisms are used to study	3N-6	3N-5	3N-3	3N			3N-5
When two different frequencies of laser are used to study raman spectrum of a sample, it wa	reflection	total internal reflection	diffraction	interference			diffraction
The vibrational energy of a molecule when it is in the lowest vibrational level is known as	UV spectrum	IR spectrum	microwave spectrum	Electronic spectrum			IR spectrum
The value of the zero point energy is ----- where n0 is the frequency of the fundamental mod	these lines are not due to rama	these lines are also part of r	these lines are IR lines	none of the above			these lines are not due to raman scattering
The vibrational transition between v=0 to v=1 isknown as	potential energy	zero point energy	knetic energy	none of the above			zero point energy
In the case of carbon dioxide, symmetric stretching is	1/2 n0	n0	2n0	1/4 n0			1/2 n0
Resonance raman scattering occurs when	fundamental	first overtone	second overtone	hot band			fundamental
Far infrared region ranges from	raman active & IR inactive	raman active and IR active	raman inactive and IR ac	raman inactive and IR inactive			raman active & IR inactive
When vibrational quantum number increases, the separation between vibrational levels	rotational level coincides with	electronic level coincides w	virtual energy level coinc	none of the above			virtual energy level coincides with original level
In vibration-rotation IR spectra, the selection rule for P-branch of lines is	4000 to 400 cm^-1	400 to 50 cm^-1	12500 to 4000 cm^-1	none of the above			4000 to 400 cm^-1
The raman lines with frequency less than the exciting frequency are known as	increases	decreases	nemains the same	none of the above			increases
Polarized raman spectra can be given by	dJ=+1	dJ=-1	dJ=0	dJ=+ or -1			dJ=+1
In IR absorption spectra, the region between -------- is called as finger print region	Rayleigh lines	stokes lines	antistokes lines	resonance lines			Rayleigh lines
In the case of water molecule all the three modes of vibrations are	single crystals only	liquids only	powder samples only	both single crystals and powder samples			single crystals only
FTIR is normally used to study	less than 900 cm^-1	between 900 and 1450 cm^	1450 to 5000 cm^-1	above 5000 cm^-1			between 900 and 1450 cm^-1
Laser used for Raman studies mainly due to its	IR and Raman active	IR active and Raman inactiv	IR inactive and Raman ac	IR inactive and Raman inactive			IR and Raman active
Conventional spectroscopy, where intensity is recorded with frquency is called	far infrared spectrum	near IR spectrum	middle IR spectrum	all the above			far infrared spectrum
Most common method of sample handling method for IR studies of solids is	coherence	high intensity	monochromaticity	directionality			middle IR spectrum
Thermocouple is used as detector in ----- spectrometer	time domain spectroscopy	frequency domain spectrosc	intensity spectroscopy	none of the above			high intensity
The most common detector in a laser Raman spectrometer is -----	pellet technique	mull technique	thin film technique	none of the above			pellet technique
In FTIR technique, normally, the signal is converted from -----	Raman	Microwave	IR	NMR			IR
Most intense IR absorption line is the one originating from v =	bolometer	thermocouple	photographic film	photomultiplier tube			photomultiplier tube
The anhamonicity of vibration of a diatomic molecule is due to	time domail to frequency doma	frequency domain to time d	frequency to intensity	none of the above			time domail to frequency domain
The virtual energy level in the case of Raman spectra is -----	1	2	0	3			0
Rayleigh scattering is	rigid nature of the bond	non-rigid nature of the bonc	due to the charge of the	due to the mass of the atoms			rigid nature of the bond
In Raman spectra, anti-Stokes lines are	characteristic of the molecule	a combined effect of the mc	depends only on the incic	none of the above			characteristic of the molecule
The stokes lines of Raman spectra are	inelastic process	elastic process	collision process	none of the above			inelastic process
Raman spectra can be obtained from	red shifted	blue shifted	no change	can be either red shifted or blue shifted			red shifted
In the case of molecules of centre of symmetry, the Raman active modes are not IR active an	red shifted	blue shifted	no change	can be either red shifted or blue shifted			red shifted
The polarisability ellipsoid of a linear molecule is	solids only	liquids only	gases only	solids, liquids and gases			solids, liquids and gases
The branch of rotational IR lines with selection rule dJ = 0 is called	Pauli's exclusion principle	Frank Condon principle	Mutual exclusion princip	none of the above			Mutual exclusion principle
Raman effect supports	elliptical	spherical	ellipsoid	none of the above			spherical
In Raman spectrum, if λ is the wavelength of incident radiation, then the Anti-Stoke's lines w	Q branch	P branch	R branch	S branch			Q branch
Sun appears red at sun rise and sunset. This is due to scattering of	corpuscular theory	wave theory	quantum theory	electromagnetic theory			quantum theory
In Raman spectrum, if λ is the wavelength of incident radiation, then the Stoke's lines will ha	λ	λ + Δλ	λ - Δλ	λ2			λ - Δλ
Tyndall effect is the scattering of the light by	longer wavelengths	shorter wavelengths	lower frequencies	all frequencies			shorter wavelengths
In 1928,Sir C.V.Raman was studying the	λ	λ + Δλ	λ - Δλ	λ2			λ + Δλ
Coefficient of scattering of light in any medium is inversely proportional to the fourth power	air particles	solid particles	liquid particles	colloidal particles			colloidal particles
Raman lines had frequencies lower than that of the incident line are called	diffraction of light	interference	scattering of light	reflection of light			scattering of light
Raman lines had frequencies higher than that of the incident line are called	wavelength of light	frequency of light	velocity of light	none of these			wavelength of light
Low frequency side and high frequency side Raman lines are referred to as	stokes lines	antistokes lines	both a and b	excitation line			stokes lines
In Rayleigh scattering, there is a change in the intensity of the scattered light, there is no cha	stokes lines	antistokes lines	both a and b	excitation line			antistokes lines
Rayleigh scattering is also called	stokes lines	antistokes lines	stokes and antistokes lin	unmodified line			stokes and antistokes lines respectively
Light from a helium discharge tube filtered by nickel oxide glass gives a light of wavelength	spectral character	wavelength	frequency	all the above			all the above
The apparatus used in the study of Raman effect in liquids was first designed by	incoherent scattering	coherent scattering	diffraction	compton scattering			coherent scattering
Raman got nobel prize in	3880Å	3888Å	3800Å	4888Å			3888Å
The modified frequencies observed in the scattering process was given the name	Wood	Rayleigh	Raman	Newton			Wood
Quinine sulphate solution contained in a novial glass vessel is used as a filter to obtain the lir	1939	1932	1931	1930			1930
Which filter is found to be a very satisfactory to get 4046Å	Compton effect	Raman effect	Scattering effect	Rayleigh scattering			Raman effect
The mercury arc is placed as close to the Raman tube as possible, which results in a large	4350Å	4340Å	4300Å	4358Å			4358Å
Which reflector is used to enhance the intensity of illumination still further	a solution of iodine in carbon t	quinine sulphate solution	nickel oxide glass	Copper oxide			a solution of iodine in carbon tetrachloride
The chief features of a spectrograph, suited for the study of Raman spectra are	intensity of the incident light	frequency of incident light	wavelength of the incide	velocity of the incident light			intensity of the incident light
The recording of the complete spectrum may require up to ten to fifteen hours, depending la	semi-cylindrical aluminium	quartz	glass	none of these			semi-cylindrical aluminium
Which is available as transparent blocks	large light gathering power	special prisms of high resolv	a short focus camera	all the above			all the above
Which of the following substance does not require container for the excitation of Raman effe	intensity of the incident light	the speed of the spectrogra	the intrinsic brilliance of	all the above			all the above
Raman effect can be obtained with solids which are in the form of loose crystal powders wa	gypsum	quartz	a & b	benzene			a & b
A special type of spectrograph with two parts, each part having a prism and two lenses with	gypsum	quartz	a & b	benzene			a & b
In the case of gases, the intensity of the light scattered is normally	Baer & Menzies	Ananthakrishnan	Billroth,Kohlrausch & Rei	Raman			Baer & Menzies
In the case of gases, wood employed a very long tube of	Baer & Menzies	Ananthakrishnan	Billroth,Kohlrausch & Rei	Raman			Billroth,Kohlrausch & Reitz
Who was the first to develop the technique of exciting Raman effect in gases under high pre	very weak	very strong	medium strong	weak			very weak
Rosetti was able to obtain the Raman spectra of several gases under pressure with the	Calcite	Benzene	carbon tetrachloride	HCL gas			HCL gas
Bhagavantam has constructed a Raman tube for gases which can stand pressures upto	Baer & Menzies	Ananthakrishnan	Rosetti	Raman			Rosetti
Who obtained good spectrographs of Raman spectra of gases using the 3650Å,4046Å & 435	2500Å line	2537Å line	2530Å line	2535Å line			2537Å line
Raman effect has been observed & studied in	30 atmospheres	40 atmospheres	50 atmospheres	60 atmospheres			50 atmospheres
With benzene, the frequency shifts of the Raman lines correspond to an infra-red wavelengt	Baer & Menzies	Ananthakrishnan	Bhagavantam	Raman			Bhagavantam
In absorption spectrum, benzene exhibits a	solids	liquids	gases	all the above			all the above
The triad of stokes and antistokes lines equally spaced on either side of the exciting 4358Å li	3µ	3.27µ	3.5µ	4µ			3.27µ
What bands are found in well purified water	weak band	medium strong band	strong band	sharp band			strong band
Solutions of salts in water give Raman spectra characteristic of the	Calcite	Benzene	carbon tetrachloride	HCL gas			carbon tetrachloride
The frequency shift of the Raman line of HCl gas corresponds to	two broad bands	one broad band	sharp band	weak band			two broad bands
Which shows the frequency shift equal to the frequency of Infra-red bands	only salts	only water	both salts and water	either salts or water			both salts and water
Which of the following gas shows a frequency shift equal to the frequency difference of two	3µ	3.27µ	3.46µ	4µ			3.46µ
The Raman lines obtained with crystals are sharp, becoming diffuse with rise of	HCl	carbondioxide	carbonmonoxide	oxygen			carbonmonoxide
The two lines exist nearest to the exciting line have been identified with the oscillations of th	HCl	carbondioxide	carbonmonoxide	oxygen			carbondioxide
Diamond exhibits a	intensity of the incident light	frequency	velocity	temperature			temperature
All the Raman lines move inward towards the parent line with	calcite	diamond	HCl	water			calcite
The variations in intensity are of great significance in the study of	broad line	very strong line	very sharp line	strong and sharp line			strong and sharp line
Which is used to separate the vertical and horizontal components in the scattered light	decrease of temperature	increase of temperature	increase of intensity	decrease of intensity			increase of temperature
Crystalline quartz should not be used for	molecular structure	chemical constitution	shape and size	both a and b			both a and b
Menzies has investigated the polarisation of the Raman lines in	quartz crystal	calcite	double image prism	suitably oriented double image prism			suitably oriented double image prism
For the vibrational Raman lines, the depolarisation factor varies from	condenser	spectrographs	windows	all the above			all the above
A simple and satisfactory explanation on the quantum theory was put forwar by	solids	liquids	gases	all the above			liquids
Which would result in the appearance of the unmodified line in the scattered beam	0 to 0.86	0 to 0.70	0 to 0.80	0 to 0.60			0 to 0.86
The frequency shift is the	Sir C.V.Raman	Prof.Smekal	Rayleigh	Bhagavantam			Prof.Smekal
Raman spectra are determined by	The photon without absorbing	absorb part of the energy of	molecule imparts some c	all the above			The photon without absorbing energy
Carbon dioxide has two very strong bands in the infra-red absorption spectrum at	difference between stokes and	difference between the inci	addition between the inc	any of the above			difference between the incident and scattered lines
Nitrous oxide molecule has the same number of electrons as	the number of atoms in the mc	the masses of the atoms	the strength of the chem	all the above			all the above
The band at 589cm-1 has not been recorded in the Raman spectrum of nitrous oxide due to	668 and 2349 cm-1	600 and 3349 cm-1	700 and 2349 cm-1	668 and 2900 cm-1			668 and 2349 cm-1
nitrous oxide has a	CO2	CO	water	carbon disulphide			CO2
According to theory, all triatomic molecules of bent symmetrical structure should give rise t	weak frequency	weak intensity	strong intensity	strong frequency			weak intensity
Depolarization factor is the ratio of the	unsymmetrical structure	symmetrical structure	center of symmetry	either a or b			unsymmetrical structure
The natural frequency of vibration is given by	two Raman lines	one Raman lines	no Raman lines	three Raman lines			three Raman lines
	Frequencies of the vertical and	Frequencies of the horizont	Intensities of the horizon	Intensities of the vertical and horizontal components			Intensities of the horizontal and vertical components
	v=1/2π(F)^1/2	v=1/2π(F/µ)^1/2	v=(F/µ)^1/2	v=1/2π(µ/F)^1/2			v=1/2π(F/µ)^1/2

SYLLABUS

Hydrogen spectra – Angular momentum – Larmor precession – Spin-orbit interactions - Spectra of alkali metals – Energy level and spectral transitions of Helium - Normal Zeeman effect – Anomalous Zeeman effect – Paschen back effect – Inference of nuclear spin - Hyperfine structure of spectral lines – Stark effect – Characteristic X-ray spectra

Classification of molecules – Interaction of radiation with rotating molecule – Rotational spectra of rigid diatomic molecule – Isotopic effect – Non-rigid rotator – Linear, symmetric and asymmetric top molecules – Quadrapole hyperfine interaction – Microwave spectrometer

Hydrogen Spectrum Definition

A Hydrogen atom consists of only one proton and the electron that revolves in the electron cloud. The emission spectrum of Hydrogen is observed when the Hydrogen molecule breaks up into Hydrogen atoms and the electrons present in them are promoted to higher energy levels. The transition of electrons between the energy levels gives out a spectrum and hence the name. The Hydrogen spectrum is relatively simple and understandable easily as compared to other elements.

Hydrogen Spectrum Series

The complete spectrum of Hydrogen consists of separate series of distinct wavelengths concentrated in the ultra violet, visible and Infra-red regions of the electromagnetic spectrum. The six series found are named after their discoverers. In the order of increasing wavelength they are the Lyman series (ultra violet), Balmer series (visible), Paschen series, Brackett series, Pfund series, and Humphrey’s series (infra-red).Each of these series is called line spectrum because the images in spectrometer appears as a pattern of thin vertical lines.The Hydrogen emits a red- violet characteristic colour. This light when passed through a prism shows four separate lines in the visible range. These are Hα, Hβ, Hϒ, and Hδ. This is the spectrum of Balmer series for Hydrogen.

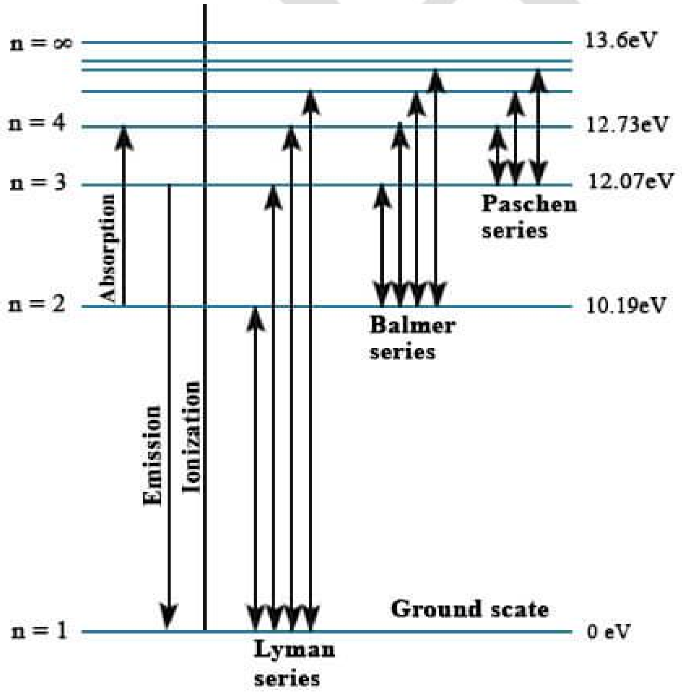
These individual lines become more closely spaced in a regular way as we get to see from longer to shorter wavelengths.

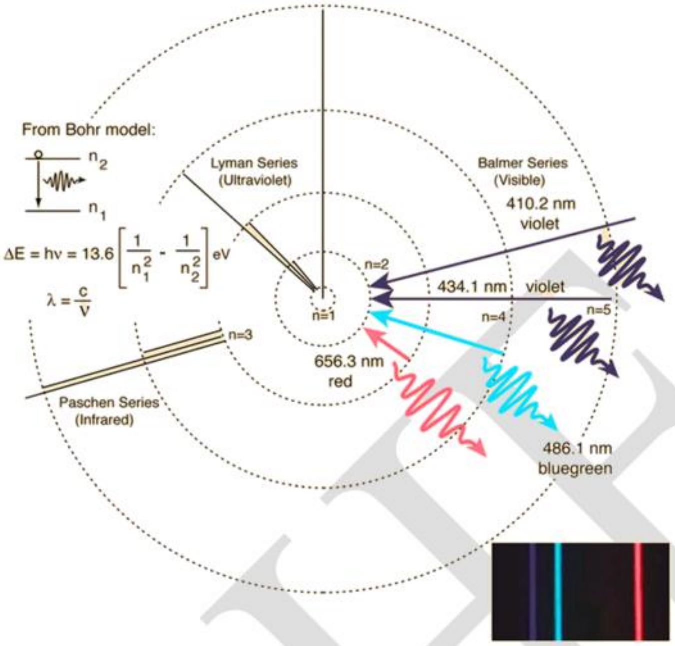
Mathematical representation,

$$\frac{1}{\lambda} = \nu = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Where, λ is wavelength in meters, ν is the wave number, R_H is Rydberg constant (10967758 per meter) and n the series of integers.

Hydrogen Spectrum Diagram





This spectrum was produced by exciting a glass tube of hydrogen gas with about 5000 volts from a transformer. It was viewed through a diffraction grating with 600 lines/mm. The colors cannot be expected to be accurate because of differences in display devices.

Lyman Series of Hydrogen Spectrum

Bohr labelled each of the energy levels in Hydrogen atom with principle quantum number n. In any Hydrogen atom which is not in an excited level, the electron is in the energy level n = 1. This state of lowest energy for the atom is called the ground state.Bohr also showed that the series in high energy ultra violet region or the Lyman series arises from electronic transition from higher energy levels to the energy level **n = 1.** Each line in the Lyman series is due to electrons returning from a particular higher energy level to the level n = 1.

Balmer Series of Hydrogen Spectrum

Almost a century ago the wavelengths that were discovered in the element spectrum were found to get into a set of pattern called **spectral series**. The first any of such series was discovered by J JBalmer during the study of visible part of the Hydrogen spectrum.The line with the longest wavelength of 656.3 nm is designated to Hα and followed by next wavelength of 486.3 nm which was designated to Hβ. With the decrease in wavelength, the lines are found to be closer together and weaker in intensity till the series reaches a wavelength of 346.6 nm. Beyond this wavelength, there are no further separate lines but only a faint continuous spectrum.

Balmer series contains wavelength in the visible portion of the hydrogen spectrum. The spectral lines of Hydrogen in the ultra violet and infra-red regions fall into several other series. Balmer's formula for the wavelength of this series is as follows.

$$\frac{1}{\lambda} = \nu = R_H \left(\frac{1}{2^2} - \frac{1}{n_2^2} \right)$$

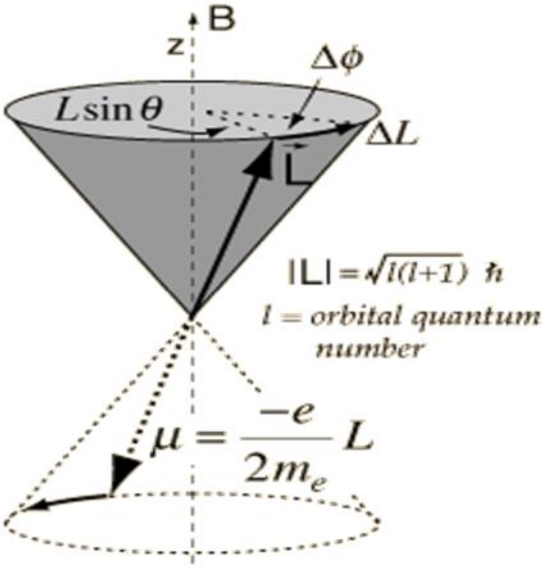
Where **R** is Rydberg constant with a value of 1.097 ×× 107 per meter and n = 3,4,5,… The Hα line corresponds to n = 3 and then Hβ line to n = 4 and so on. The series limit corresponds to n = ∞ so that this could occur at a wavelength of 4/R.

Larmor Precession

When a magnetic moment m is placed in a magnetic field B, it experiences a torque which can be expressed in the form of a vector product

$$\tau = \mu \;\; x \;\; B$$

For a static magnetic moment or a classical current loop, this torque tends to line up the magnetic moment with the magnetic field B, so this represents its lowest energy configuration. But if the magnetic moment arises from the motion of an electron in orbit around a nucleus, the magnetic moment is proportional to the angular momentum of the electron. The torque exerted then produces a change in angular momentum which is perpendicular to that angular momentum, causing the magnetic moment to precess around the direction of the magnetic field rather than settle down in the direction of the magnetic field. This is called Larmor precession.



When a torque is exerted perpendicular to the angular momentum L, it produces a change in angular momentum L which is perpendicular to L, causing it to precess about the z axis. Labeling the precession angle as , we can describe the effect of the torque as follows:

$$\tau = \frac{\Delta L}{\Delta t} = \frac{L\sin\theta\Delta\phi}{\Delta t} = |\mu B\sin\theta| = \frac{e}{2m_e} LB\sin\theta$$

The precession angular velocity (Larmor frequency) is

$$\omega_{Larmor} = \frac{d\phi}{dt} = \frac{e}{2m_e} B$$

These relationships for a finite current loop extend to the magnetic dipoles of electron orbits and to the intrinsic magnetic moment associated with electron spin. There is also a characteristic Larmor frequency for nuclear spins.

In the case of the electron spin precession, the angular frequency associated with the spin transition is usually written in the general form where   is called the gyromagetic ratio (sometimes the magnetogyric ratio). This angular frequency is associated with the "spin flip" or spin transition, involving an energy change of 2mB. An example for magnetic field 1 Tesla follows.

$$\omega_{electron\,spin} = \frac{2\mu_e B}{\hbar} = \frac{2\cdot 2\cdot \frac{1}{2}(5.79x10^{-5}eV/T)(1T)}{6.58x10^{-16}eV\cdot s} = 1.7608x10^{11}s^{-1}$$

$$\nu = \frac{\omega}{2\pi} = 28.025\,GHz \quad \textit{Larmor frequency}$$

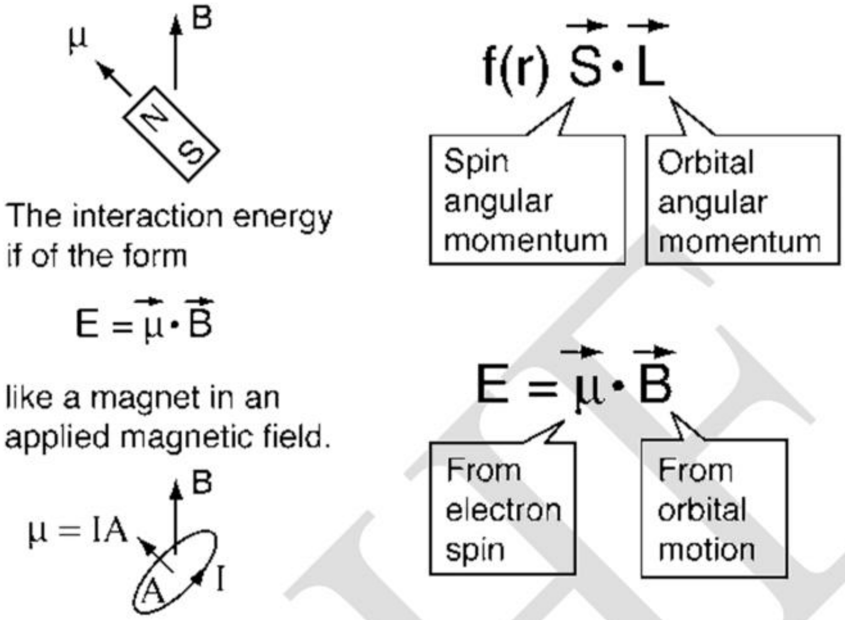
$$\omega_{proton\,spin} = \frac{2\mu_p B}{\hbar} = \frac{2(2.79)(3.15x10^{-8}eV/T)(1T)}{6.58x10^{-16}eV\cdot s} = 2.6753x10^{8}s^{-1}$$

$$\nu = \frac{\omega}{2\pi} = 42.5781\,MHz \quad \textit{Larmor frequency}$$

The characteristic frequencies associated with electron spin are employed in electron spin resonance (ESR) experiments, and those associated with the nuclear spin in nuclear magnetic resonance (NMR) experiments.

Spin-Orbit Interaction

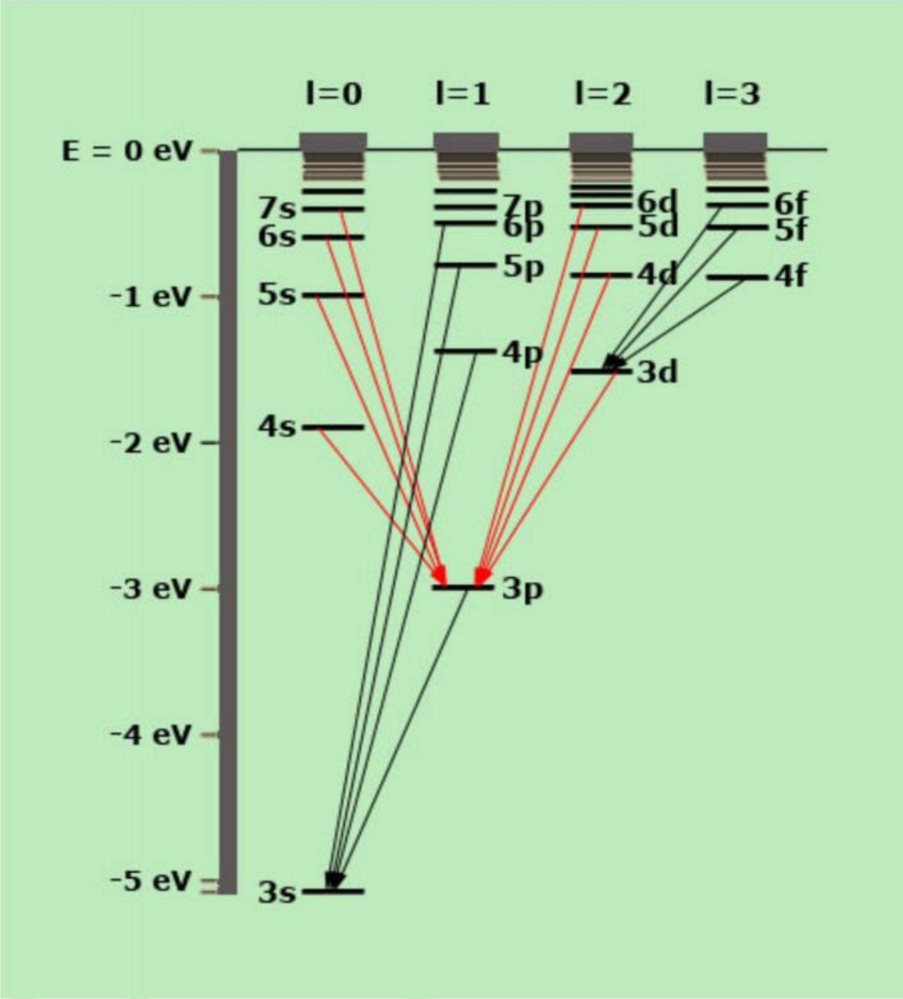
The energy levels of atomic electrons are affected by the interaction between the electron spin magnetic moment and the orbital angular momentum of the electron. It can be visualized as a magnetic field caused by the electron's orbital motion interacting with the spin magnetic moment. This effective magnetic field can be expressed in terms of the electron orbital angular momentum. The interaction energy is that of a magnetic dipole in a magnetic field and takes the form.



When atomic spectral lines are split by the application of an external magnetic field, it is called the Zeeman effect. The spin-orbit interaction is also a magnetic interaction, but with the magnetic field generated by the orbital motion of an electron within the atom itself. It has been described as an "internal Zeeman effect". The standard example is the hydrogen fine structure.

Spectra of alkali metals:

In the previous lecture we have learnt the quantum mechanical treatment of hydrogen atom. The similar picture is not able to explain the alkali atoms, the other elements in the first group of periodic table. Here, we will discuss the development of the theory to explain the alkali spectra. We will also elaborate the concept behind the modification of the potential required to explain the observation in alkali atoms. The absorption spectra of alkali vapors (Such as lithium, sodium) appear quite similar in many respects to the absorption spectrum of H atom. They are only displaced to a considerable extent, toward longer wavelengths. These spectra also consist of a series of lines with regularly decreasing separation and decreasing intensity.

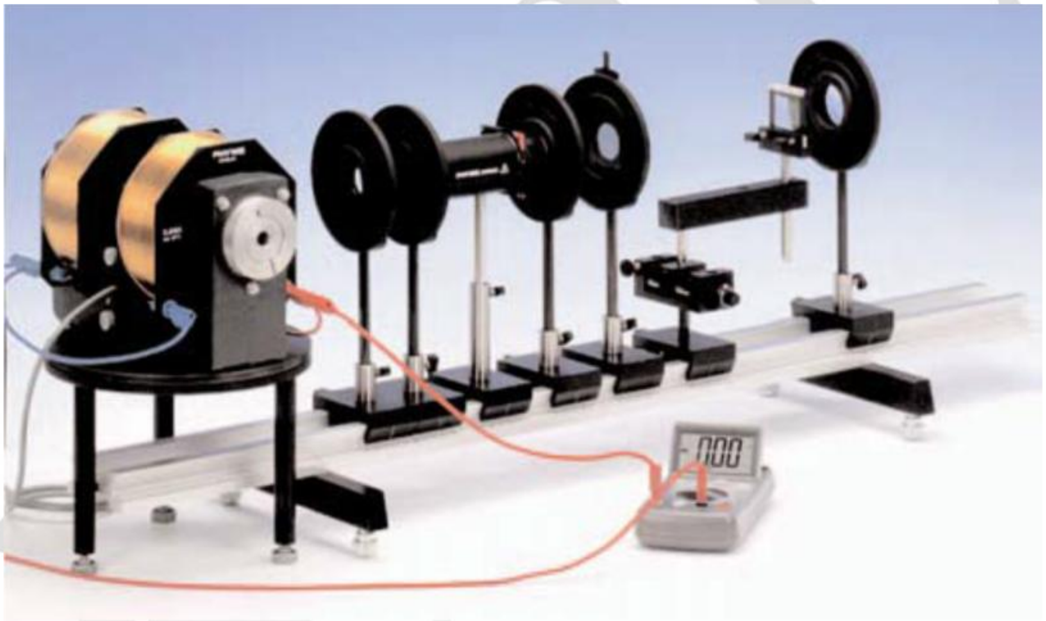


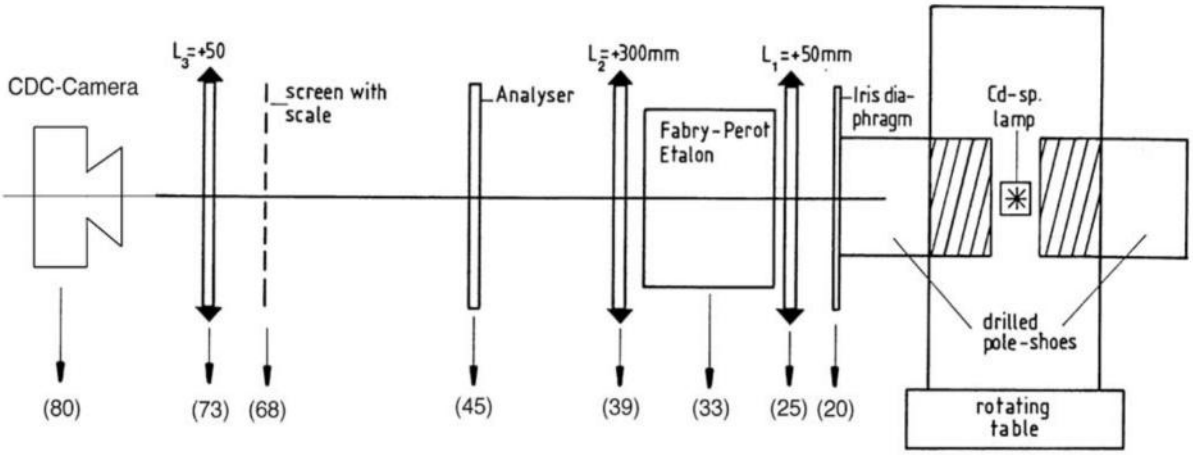
Zeeman effect:

The “Zeeman effect” is the energy shift of atomic states caused by magnetic field. This shift is due to the coupling of the electron orbital angular momentum to the external magnetic field. The normal Zeeman effect occurs when there is no spin magnetic moment – states with zero spin are necessary. In singulett systems the spins of the electrons cancel each other i.e. add up to zero. The energy shift of the atomic states in an outer magnetic field can be observed by the wavelength shift of the radiation emitted in atomic transitions between these states.

Normal Zeeman effect:

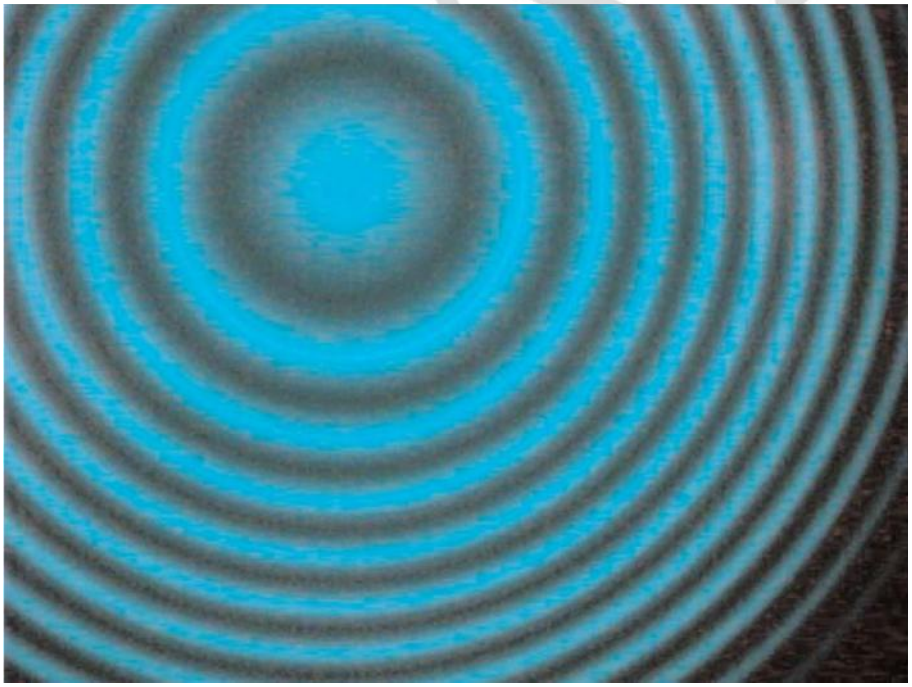
Transversal and longitudinal observation of the splitting of the red 643.847 nm Cd-line in the magnetic field showing the normal Zeeman effect. 1b. Anomalous Zeeman effect: Transversal and longitudinal observation of the splitting of the green 508.588 nm Cdline in the magnetic field showing the anomalous Zeeman effect. 2. Observation of the effect of polarization filter and polarization filter combined with l/4 plate for the splitted green and red lines in transversal and longitudinal direction. 3. Measurement of the frequency shift with help of the CCD camera and the supplied measurement software or with the screen with scale and the sliding device in the classical version for both of the above mentioned spectral lines.





Anomalous Zeeman effect:

The **anomalous Zeeman effect** is the more general case where the electron spins do not cancel each other and the energy of an atomic state in a magnetic field depends on both the magnetic moments of electron orbit and electron spin. The magnetic moment of the orbital angular momentum is as above and the magnetic moment of the spin.



Paschen back effect:

A theory of the molecular Zeeman effect in the Paschen-Back regime (PBR) was rest considered by Hill (1929), who described the splitting of molecular doublet levels for the intermediate case (a{b) using Hund's case (b) wavefunctions. However, he did not succeed in calculating the theoretical line strengths for this case. This was done much later by Schadee (1978), who repeated the analytical calculation by Hill using Hund's case (a) wave functions. He did not give details on line strength calculations, however, as the corresponding analytical expressions would have been too complicated. Both above approaches were limited to doublet states and to the Paschen-Back e®ect (PBE) on the ¯ne structure of molecular levels. Schadee's theory of the molecular PBE was successfully used to explain peculiar Stokes proles of molecular doublet transitions observed in sunspots: MgH (Berdyugina et al. 2000) and CN (Berdyugina, Solanki, & Frutiger 2001; Asensio Ramos, Trujillo Bueno, & Collados 2005).

POSSIBLE QUESTIONS

1. Define Orbital angular momentum.
2. Discuss Normal and Anomalous Zeeman effect in details.
3. What is the basic principle of microwave spectra?
4. Explain the construction and working of Microwave spectrometer with suitable examples.
5. Define Spin angular momentum.
6. Discuss Paschan Bach effect in details.
7. Explain the following
    i) Hydrogen Spectra
    ii) Influence of Nuclear spin
8. Explain a Quadrapole hyperfine interaction in details.
9. Explain the following
    i) Anomalous Zeeman effect
    ii) Paschan Bach effect
10. Explain symmetric and asymmetric top molecules with help of microwave spectra.
11. Explain the spectra of Alkali metals
12. Give a note on hyperfine structure of spectral lines
13. Explain the concept of Non-rigid rotator and Isotope effect.
14. Calculate the internal magnetic field produced by the nucleus which causes the splitting of the 3p state of sodium atom.

KARPAGAM ACADEMY OF HIGHER EDUCATION
(Under Section 3 of UGC Act 1956)
COIMBATORE – 641021
(For the candidates admitted from 2017 onwards)
DEPARTMENT OF PHYSICS
PHYSICS
SPECTROSCOPY (17PHP204)
MULTIPLE CHOICE QUESTIONS

QUESTIONS	OPTION 1	OPTION 2	OPTION 3	OPTION 4	OPTION 5	OPTION 6	ANSWER
The diagram representing the relation between the inter-nuclear distance and energy is cal							
In the case of microwave spectroscopy, the absorption takes place due to interaction between							
The source of microwave radiation in microwave spectroscopy is normally	Morse curve	frequency spectrum	modulation curve	none of the above			Morse curve
In a spectrometer, the devise used to split the spectral lines into its component frequencie	electric vector of the radiation	magnetic vector and the ele	electric vector of the rad	none of the above			electric vector of the radiation and magnetic dipole moment
The most commonly used and most efficient monochromator is a spectrometer is	laser	mercury vapour lap	sodium vapour lamp	klystron			klystron
The Morse curve depicts the variation of	divider	selector	monochromator	recorder			monochromator
Which of the following statements is correct?	prism	lens	diffraction grating	none of the above			diffraction grating
Electronic spectra is given by	internuclear distance with ene	energy with internuclear dis	vibraitonal energy with i	none of the above			vibraitonal energy with internuclear distance
The change in vibrational quantum numbe acoompanying an electronic transition	In a molecule, each electronic	In a molecule, each vibratio	In a molecule, each elect	In a molecule, each rotational level contains many vibrational			In a molecule, each electronic level contains many vibrational levels and each vibrational level contains many rotational levels
In fluorescence, the frequency of emitted radiation is ----- that of incident radiation	all molecules	only molecules with electric	only molecules with mag	only molecules with both electric and magnetic moments			all molecules
The emission of radiation which may last for some time even after the removal of the excit	has selection rule dv=0	has a selection rule dv = + o	has selection rule dv=0,	is not governed by any selection rule			is not governed by any selection rule
During electronic transition in a molecule the radiation normally fall in the	higher than	lower than	same as	higher or lower than			lower than
The condition for a molecule to give electronic spectra is	coherence	resonance	fluorescence	phosphorescence			phosphorescence
Electronic spectra may contain	visible region	IR region	Microwave region	UV region			visible region
During an electronic transtion, the internuclear distance remains the same. This is called	it should possess permanent e	it sould possess permanent	it should possess both p	there is no such condition			there is no such condition
The intensity distribution of vibrational lines of electronic spectra is given by using	vibrational and rotational stru	only vibrational structure	only rotational structure	no such components			vibrational and rotational structure
The absorption and emission energy in the range 10 to about 10000 angstrom is restricted	mutual exclusion principle	Frank Condon principle	Deslander's principle	none of the above			Frank Condon principle
The group of lines resulting from transitions between the different rotational levels in two	Deslander's table	Frank Condon principle	Population consideratio	none of the above			Frank Condon principle
The time required for electronic transitions is about	electronic energy	vibrational energy	rotational enegy	translational energy			electronic energy
The sum of all bands for transitions between two electronic levels is termed as	band	spectrum	spectral lines	none of the above			band
During electronic transtions the internuclear distance	10^-16 seconds	10^-14 seconds	10^-16 milliseconds	A few seconds			10^-16 seconds
The P and R branches of spectral lines are represented by a diagram called	band origin	band system	band head	band lines			band system
For all electronic levels for which the electrons are paired, the spin is ----- and multiplicity is	increases	decreases	remains the same	none of the above			remains the same
In triplet state, the probability of two electrons occuppying same state is	condon parabola	Fortrat parabola	Morse curve	none of the above			Fortrat parabola
If during a spectral emission, the electron undergoing the transition does not change its spi	1 and 0	0 and 1	0 and 0	1 and 1			0 and 1
The emission process in which the electron taking part in the emission undergoes a change	0	1	0.5	0.75			0
The process in which there occurs a delay between absorption and emission, but no chang	fluorescence	phosphorescence	scattering	raman shift			fluorescence
Emission is a spontaneous process, generally, and absorption is a ----	fluorescence	phosphorescence	delayed fluorescence	none of the above			phosphorescence
The diagram representing transitions between the various electronic and vibraitonal states	fluorescence	phosphorescence	delayed fluorescence	raman shift			delayed fluorescence
In any non-degenerate molecular orbital, only two electrons of opposite spin can be accom	stimulated	spontaneous	scattering	none of the above			stimulated
The study of the physical and chemical properties of electronically excited atoms and mole	Fortrat parabola	Condon parabola	Morse curve	Jablonski diagram			Jablonski diagram
Which of the following statements is correct?	Pauli's exclusion principle	Frank Condon principle	Mutual exclusion princip	none of the above			Pauli's exclusion principle
Some of the electronically excited states undego	Physical chemistry	photochemistry	photonics	electrolysis			Physical chemistry
Fluorescence is a process in which the electron -----	All electronically excited states	All electronicaly excited sta	None of the electronicall	All electronically excited states undergo stimulated emission			All electronicaly excited states do not give rise to observable emission
The principle involved in scintillators is	relaxation	absorption	scattering	collision			relaxation
Fluorescence emission is a ------ process	emits energy as radiation and	emits energy as radiation a	does not emit energy as	does not emit energy as radiation and does not undergo chan			emits energy as radiation and does not undego change in spin
The process in which absorbed radiation is not emitted as radiation is called	phosphorescence	fluorescence	delayed fluorescence	ionisation			fluorescence
The electronic spectra fall within the range	stimulated	scattering	spontaneous	none of the above			spontaneous
Frank Condon principle states that during an electronic transition, the internucluear distanc	spontaneous emission	stimulated emission	scattering	non-radiative transfer			non-radiative transfer
The triplet state is always ----- in energy than the corresponding state	10 to 10000 asgstrom	4000 to 12500 angstrom	50 to 400 cm^-1	none of the above			10 to 10000 asgstrom
The electronic transition is spin forbidden, if the initial and final states have	changes	does not change	becomes double	becomes half			does not change
At very low pressures in the vapour phase, the electronically excited molecules may not su	higher	equal	lower	none of the above			lower
Fortrat parabola represents ----- , represented by v - m plot	same multiplicity	different multiplicity	less multiplicity	none of the above			different multiplicity
If a molecule is excited to some vibrational level of S1 state under high pressure, the initiall	normal fluorescence	delayed fluorescence	resonance fluorescence	phosphorescence			normal fluorescence
The difference in position of maximum of emission and of zero-zero transition on an energ	The P and R branches	P branche only	R branch only	S branch only			The P and R branches
	normal fluorescence	delayed fluorescence	resonance fluorescence	phosphorescence			normal fluorescence
	Stokes loss	anti stokes loss	collision loss	none of the above			anti stokes loss

SYLLABUS

Quantum mechanical and Classical description - The Bloch equation - Relaxation process - the experimental technique - Principle and working of high resolution NMR Spectrometer - Chemical shift – Applications of NMR
Fundamental requirements - General principle - Experimental detection of NQR frequencies – Interpretation and chemical explanation of NQR spectroscopy – Applications of NQR

Nuclear Magnetic Resonance Spectroscopy

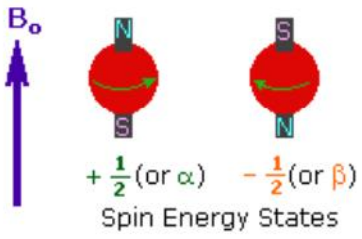
Background

Over the past fifty years nuclear magnetic resonance spectroscopy, commonly referred to as nmr, has become the preeminent technique for determining the structure of organic compounds. Of all the spectroscopic methods, it is the only one for which a complete analysis and interpretation of the entire spectrum is normally expected. Although larger amounts of sample are needed than for mass spectroscopy, nmr is non-destructive, and with modern instruments good data may be obtained from samples weighing less than a milligram. To be successful in using nmr as an analytical tool, it is necessary to understand the physical principles on which the methods are based.

The nuclei of many elemental isotopes have a characteristic spin (**I**). Some nuclei have integral spins (e.g. I = 1, 2, 3 ....), some have fractional spins (e.g. I = 1/2, 3/2, 5/2 ....), and a few have no spin, I = 0 (e.g. 12C, 16O, 32S, ...). Isotopes of particular interest and use to organic chemists are 1H, 13C, 19F and 31P, all of which have I = 1/2. Since the analysis of this spin state is fairly straight foreward, our discussion of NMR will be limited to these and other I = 1/2 nuclei.

The following features lead to the NMR phenomenon:

1. A spinning charge generates a magnetic field, as shown by the animation on the right. The resulting spin-magnet has a magnetic moment (**μ**) proportional to the spin.
2. In the presence of an external magnetic field (**B0**), two spin states exist, **+1/2** and **-1/2**. The magnetic moment of the lower energy +1/2 state is aligned with the external field, but that of the higher energy -1/2 spin state is opposed to the external field. Note that the arrow representing the external field points North.
3. The difference in energy between the two spin states is dependent on the external magnetic field strength, and is always very small. The following diagram illustrates that the two spin states have the same energy when the external field is zero, but diverge as the field increases. At a field equal to Bx a formula for the energy difference is given (remember I = 1/2 and μ is the magnetic moment of the nucleus in the field).

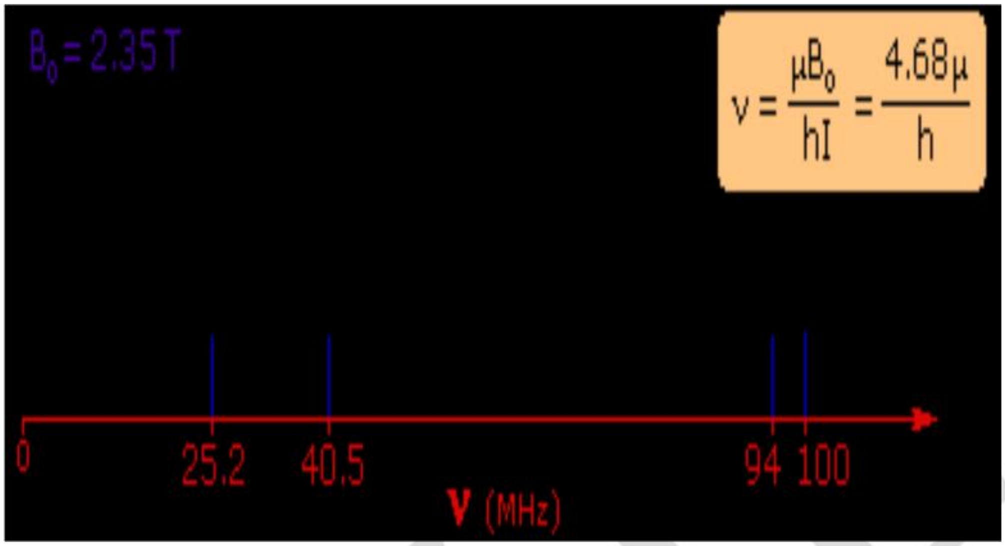


Strong magnetic fields are necessary for nmr spectroscopy. The international unit for magnetic flux is the tesla (**T**). The earth's magnetic field is not constant, but is approximately 10-

4 T at ground level. Modern nmr spectrometers use powerful magnets having fields of 1 to 20 T. Even with these high fields, the energy difference between the two spin states is less than 0.1 cal/mole. To put this in perspective, recall that infrared transitions involve 1 to 10 kcal/mole and electronic transitions are nearly 100 time greater. For nmr purposes, this small energy difference (ΔE) is usually given as a frequency in units of MHz (106 Hz), ranging from 20 to 900 Mz, depending on the magnetic field strength and the specific nucleus being studied. Irradiation of a sample with radio frequency (rf) energy corresponding exactly to the spin state separation of a specific set of nuclei will cause excitation of those nuclei in the +1/2 state to the higher -1/2 spin state. Note that this electromagnetic radiation falls in the radio and television broadcast spectrum. Nmr spectroscopy is therefore the energetically mildest probe used to examine the structure of molecules. The nucleus of a hydrogen atom (the proton) has a magnetic moment μ = 2.7927, and has been studied more than any other nucleus. The previous diagram may be changed to display energy difference

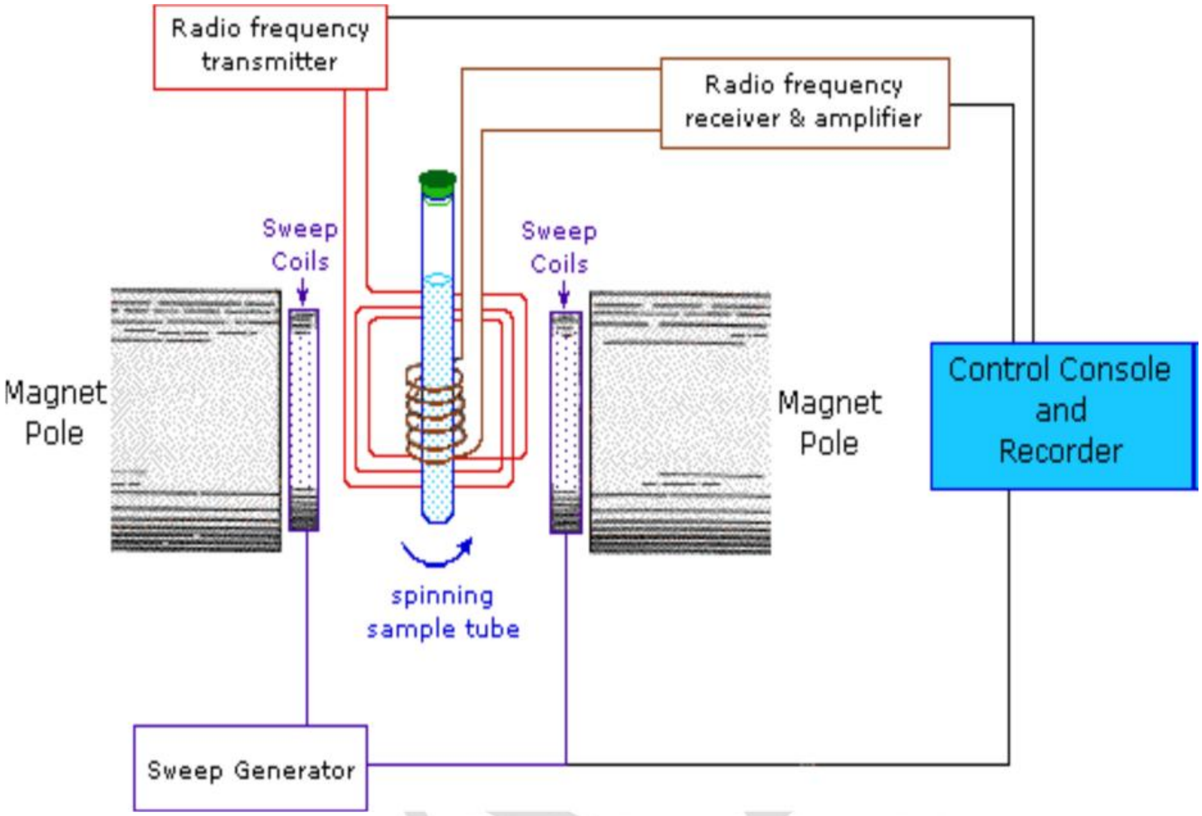
For spin 1/2 nuclei the energy difference between the two spin states at a given magnetic field strength will be proportional to their magnetic moments. For the four common nuclei noted above, the magnetic moments are: 1H μ = 2.7927, 19F μ = 2.6273, 31P μ = 1.1305 & 13C μ = 0.7022. These moments are in nuclear magnetos, which are 5.05078•10-27 JT-1. The following diagram gives the approximate frequencies that correspond to the spin state energy separations for each of these nuclei in an external magnetic field of 2.35 T. The formula in the colored box shows the direct correlation of frequency (energy difference) with magnetic moment (h = Planck's constant = 6.626069•10-34 Js).

s for the proton spin states (as frequencies) by mouse clicking anywhere within it.

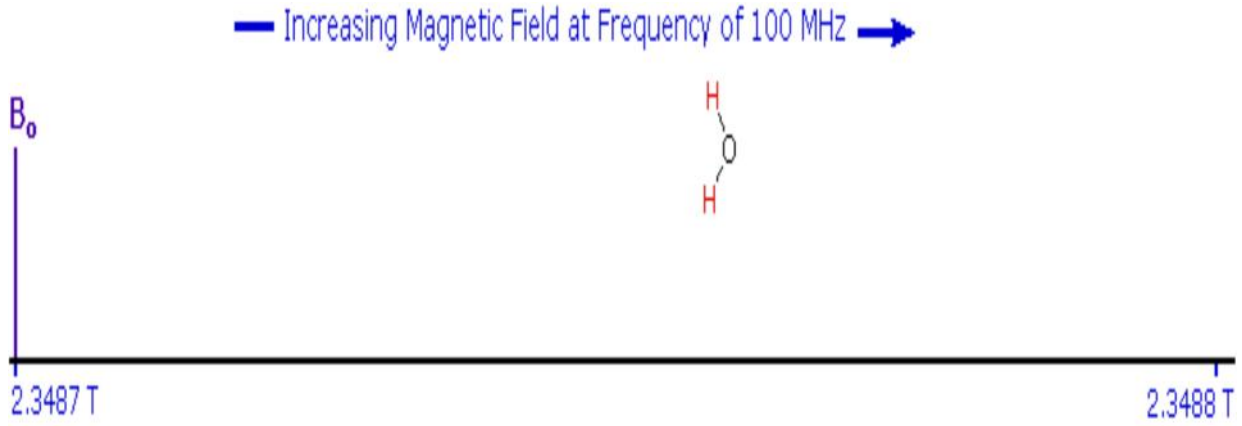


Proton NMR Spectroscopy

This important and well-established application of nuclear magnetic resonance will serve to illustrate some of the novel aspects of this method. To begin with, the nmr spectrometer must be tuned to a specific nucleus, in this case the proton. The actual procedure for obtaining the spectrum varies, but the simplest is referred to as the continuous wave (CW) method. A typical CW-spectrometer is shown in the following diagram. A solution of the sample in a uniform 5 mm glass tube is oriented between the poles of a powerful magnet, and is spun to average any magnetic field variations, as well as tube imperfections. Radio frequency radiation of appropriate energy is broadcast into the sample from an antenna coil (colored red). A receiver coil surrounds the sample tube, and emission of absorbed RF energy is monitored by dedicated electronic devices and a computer. An NMR spectrum is acquired by varying or sweeping the magnetic field over a small range while observing the rf signal from the sample. An equally effective technique is to vary the frequency of the rf radiation while holding the external field constant.



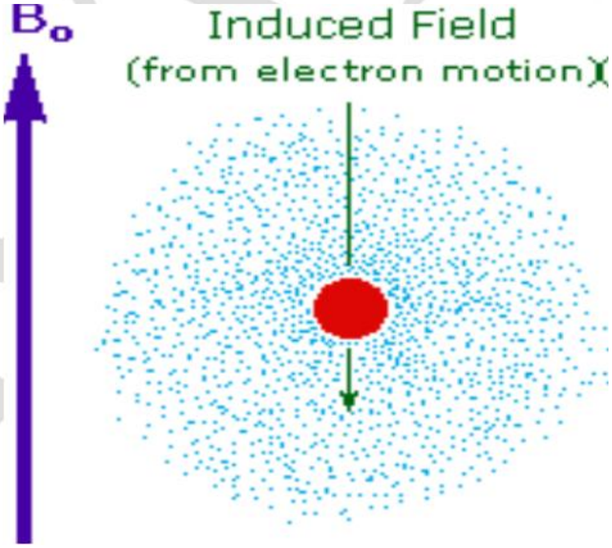
As an example, consider a sample of water in a 2.3487 T external magnetic field, irradiated by 100 MHz radiation. If the magnetic field is smoothly increased to 2.3488 T, the hydrogen nuclei of the water molecules will at some point absorb rf energy and a resonance signal will appear. An animation showing this may be activated by clicking the Show Field Sweep button. The field sweep will be repeated three times, and the resulting resonance trace is colored red. For visibility, the water proton signal displayed in the animation is much broader than it would be in an actual experiment.



Since protons all have the same magnetic moment, we might expect all hydrogen atoms to give resonance signals at the same field / frequency values. Fortunately for chemistry applications, this is not true. By clicking the Show Different Protons button under the diagram, a number of representative proton signals will be displayed over the same magnetic field range. It is not possible, of course, to examine isolated protons in the spectrometer described above; but from independent measurement and calculation it has been determined that a naked proton would resonate at a lower field strength than the nuclei of covalently bonded hydrogens. With the exception of water, chloroform and sulfuric acid, which are examined as liquids, all the other compounds are measured as gases.

Why should the proton nuclei in different compounds behave differently in the nmr experiment?

The answer to this question lies with the electron(s) surrounding the proton in covalent compounds and ions. Since electrons are charged particles, they move in response to the external magnetic field (Bo) so as to generate a secondary field that opposes the much stronger applied field. This secondary field **shields** the nucleus from the applied field, so Bo must be increased in order to achieve resonance (absorption of rf energy). As illustrated in the drawing on the right, Bo must be increased to compensate for the induced shielding field. In the upper diagram, those compounds that give resonance signals at the higher field side of the diagram (CH4, HCl, HBr and HI) have proton nuclei that are more shielded than those on the lower field (left) side of the diagram. The magnetic field range displayed in the above diagram is very small compared with the actual field strength (only about 0.0042%). It is customary to refer to small increments such as this in units of parts per million (ppm). The difference between 2.3487 T and 2.3488 T is therefore about 42 ppm. Instead of designating a range of NMR signals in terms of magnetic field differences (as above), it is more common to use a frequency scale, even though the spectrometer may operate by sweeping the magnetic field. Using this terminology, we would find that at 2.34 T the proton signals shown above extend over a 4,200 Hz range (for a 100 MHz rf frequency, 42 ppm is 4,200 Hz). Most organic compounds exhibit proton resonances that fall within a 12 ppm range (the shaded area), and it is therefore necessary to use very sensitive and precise spectrometers to resolve structurally distinct sets of hydrogen atoms within this narrow range. In this respect it might be noted that the detection of a part-per-million difference is equivalent to detecting a 1 millimeter difference in distances kilometer.



Chemical Shift

Unlike infrared and uv-visible spectroscopy, where absorption peaks are uniquely located by a frequency or wavelength, the location of different NMR resonance signals is dependent on both the external magnetic field strength and the RF frequency. Since no two magnets will have exactly the same field, resonance frequencies will vary accordingly and an alternative method for characterising and specifying the location of NMR signals is needed. This problem is illustrated by the eleven different compounds shown in the following diagram. Although the eleven resonance signals are distinct and well separated, an unambiguous numerical locator cannot be directly assigned to each.

One method of solving this problem is to report the location of an NMR signal in a spectrum relative to a reference signal from a standard compound added to the sample. Such a reference standard should be chemically unreactive, and easily removed from the sample after the measurement. Also, it should give a single sharp NMR signal that does not interfere with the resonances normally observed forganic compounds. Tetramethylsilane, $(CH_3)_4Si$, usually referred to as TMS, meets all these characteristics, and has become the reference compound of choice for proton and carbon NMR. Since the separation (or dispersion) of nmr signals is magnetic field dependent, one additional step must be taken in order to provide an unambiguous location unit. This is illustrated for the acetone, methylene chloride and benzene signals by clicking on the previous diagram. To correct these frequency differences for their field dependence, we divide them by the spectrometer frequency (100 or 500 MHz in the example), as shown in a new display by again clicking on the diagram. The resulting number would be very small, since we are dividing Hz by MHz, so it is multiplied by a million, as shown by the formula in the blue shaded box. Note that vref is the resonant frequency of the reference signal and vsamp is the frequency of the sample signal. This operation gives a locator number called the **Chemical Shift**, having units of parts-per-million (ppm), and designated by the symbol **δ** Chemical shifts for all the compounds in the original display will be presented by a third click on the diagram.

The compounds referred to above share two common characteristics:

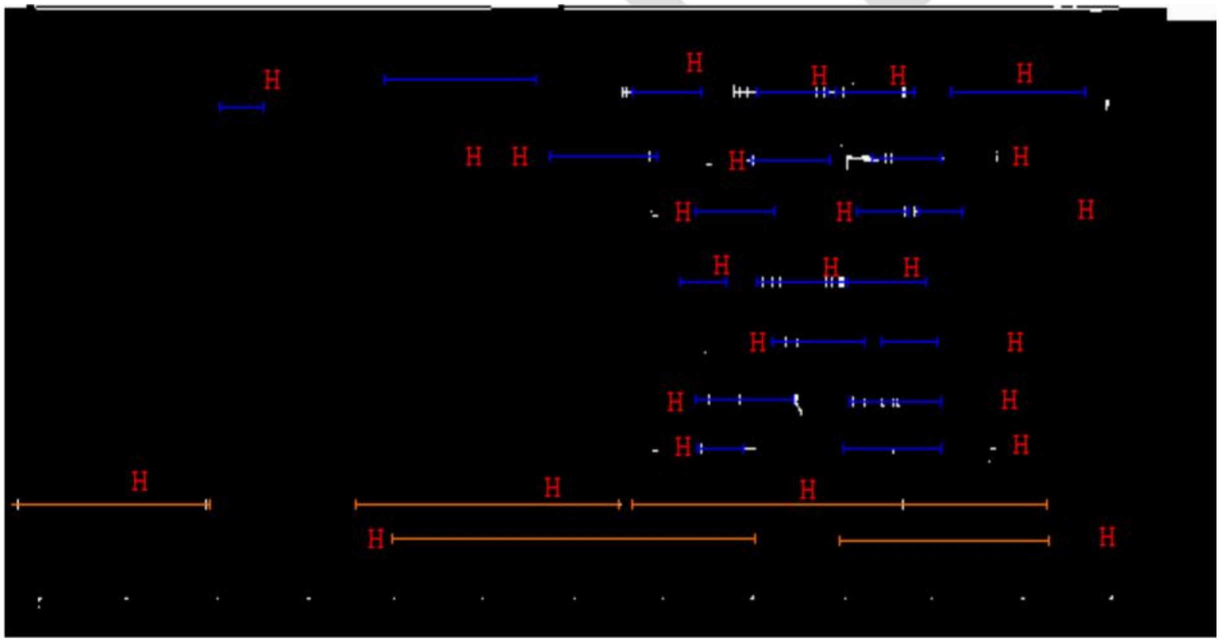
- The hydrogen atoms in a given molecule are all structurally equivalent, averaged for fast conformational equilibria.
- The compounds are all liquids, save for neopentane which boils at 9 °C and is a liquid in an ice bath.

The first feature assures that each compound gives a single sharp resonance signal. The second allows the pure (neat) substance to be poured into a sample tube and examined in a nmr spectrometer. In order to take the nmr spectra of a solid, it is usually necessary to dissolve it in a suitable solvent. Early studies used carbon tetrachloride for this purpose, since it has no hydrogen that could introduce an interfering signal. Unfortunately, CCl_4 is a poor solvent for many polar compounds and is also toxic. Deuterium labeled compounds, such as deuterium oxide (D2O), chloroform-d (DCCl3), benzene-d6 (C6D6), acetone-d6 (CD3COCD3) and DMSO-d6 (CD3SOCD3) are now widely used as nmr solvents. Since the deuterium isotope of hydrogen has a different magnetic moment and spin, it is invisible in a spectrometer tuned to protons.

From the previous discussion and examples we may deduce that one factor contributing to chemical shift differences in proton resonance is the **inductive effect**. If the electron density about a proton nucleus is relatively high, the induced field due to electron motions will be stronger than if the electron density is relatively low. The shielding effect in such high electron density cases will therefore be larger, and a higher external field (Bo) will be needed for the rf energy to excite the nuclear spin. Since silicon is less electronegative than carbon, the electron density about the methyl hydrogens in tetramethylsilane is expected to be greater than the electron density about the methyl hydrogens in neopentane (2,2-dimethylpropane), and the characteristic resonance signal from the silane derivative does indeed lie at a higher magnetic field. Such nuclei are said to be **shielded**. Elements that are more electronegative than carbon should exert an opposite effect (reduce the electron density); and, as the data in the following tables show, methyl groups bonded to such elements display lower field signals (they are deshielded). The deshielding effect of electron withdrawing groups is roughly proportional to their electronegativity, as shown by the left table. Furthermore, if more than one such group is present, the deshielding is additive (table on the right), and proton resonance is shifted even further downfield.

The general distribution of proton chemical shifts associated with different functional groups is summarized in the following chart. Bear in mind that these ranges are approximate, and may not encompass all compounds of a given class. Note also that the ranges specified for OH and NH protons (colored orange) are wider than those for most CH protons. This is due to hydrogen bonding variations at different sample concentrations.

Proton Chemical Shift Ranges



Nuclear Quadrupole Resonance Spectroscopy:

Nuclear quadrupole resonance (NQR) uses radio-frequency (RF) magnetic fields to induce and detect transitions between sublevels of a nuclear ground state, a description that also applies to nuclear magnetic resonance (NMR). NMR refers to the situation where the sublevel energy splitting is predominantly due to a nuclear interaction with an applied static magnetic field, while NQR refers to the case where the predominant splitting is due to an interaction with electric field gradients within the material. So-called “pure NQR” refers to the common case when there is no static magnetic field at all. That property may simply be the sample temperature, for use as an NQR thermometer [4, 5], or even whether or not a sample is present when NQR is used for materials detection [6]. On the other hand, NQR is also used to obtain detailed information on crystal symmetries and bonding, on changes in lattice constants with pressure, about phase transitions in solids, and other properties of materials of interest to solid state physicists and chemists.

The Nuclear Electric Quadrupole Interaction:

A non-zero electric quadrupole moment arises for nuclei that are classically described as prolate (“stretched”) or oblate (“squashed”) spheroids. The nuclear charge distribution has axial symmetry and the axis of symmetry coincides with the direction of the nuclear angular momentum and the nuclear magnetic dipole moment. In general, an electric quadrupole moment is described by a 3 - 3 symmetric, traceless tensor **Q**. For a nucleus such a tensor can be determined using a single value that describes how prolate or oblate the nucleus is, plus a description of the orientation of the nucleus. Since the charge distribution for a nucleus with spin 0 or ½ is spherical, such nuclei will have no electric quadrupole moment.

POSSIBLE QUESTIONS

1. Write a note on NMR?
2. Write a note on NQR?
3. Describe chemical shift.
4. Write about high resolution NQR spectrometer with suitable diagram.
5. Discuss about classical description of NMR spectroscopy
6. Explain the construction and working of high resolution NMR spectrometer with suitable examples.
7. Explain the construction and working of high resolution NQR spectrometer with suitable examples.
8. The ^{14}N resonance of a compound showed 3 lines at 5.997, 3.501 and 2.496 MHz. Calculate the quadrupole coupling constant e^2qQ/h and η.

KARPAGAM ACADEMY OF HIGHER EDUCATION
(Under Section 3 of UGC Act 1956)
COIMBATORE – 641021
(For the candidates admitted from 2017 onwards)
DEPARTMENT OF PHYSICS
PHYSICS
SPECTROSCOPY (18PHP204)
MULTIPLE CHOICE QUESTIONS

QUESTIONS	**OPTION 1**	**OPTION 2**	**OPTION 3**	**OPTION 4**	**OPTION 5**	**OPTION 6**	**ANSWER**
For sample to be NMR active, the spin of the nucleus must be							
In the super-regenerative NQR spectrometer, the oscillations are -----							
The NMR and NQR frequencies fall in the	equal to zero	equal to 1/2	equal to + or - 1	greater than 1/2			greater than 1/2
In NQR experiment, the frequency of the input radiation must be	insignificant	quenched	non quenched	significant			insignificant
NQR is observed normally in	radio frequency region	visible region	UV region	microwave region			radio frequency region
Nucei having ----- due to their spin, exhibit NMR spectrum	fixed	variable	can be either fixed or var	none of the above			variable
For nuclei with mass number odd and atomic number even or odd, the spin is	solids only	gas only	liquid only	in all the three			solids only
In NQR the energy levels are ----- in nature	magnetic moments	electric dipole moment	electron spin	none of the above			magnetic moments
In the equation for nuclear magnetic moment (mu)N = gamma*Ih*2pi, gamma is known as	zero	half integer	integer	can be anything			half integer
In NMR, resonance condition can be obtianed by	both electrical and megnetic	electrical	magnetic	none of these			electrical
The condition in which there is no net absorption or emission in the case of NMR is caled	nuclear quadrupole moment	electric dipole moment	gyromagnetic ratio	none of the above			gyromagnetic ratio
The condition of saturation occurs when	eiher fixed magnetic field and v	only by fixed magnetic field	only fixed frequency and	by varying both magnetic field and frequency			eiher fixed magnetic field and varying frequency, or fixed frequency and varying magnetic field
The condition of saturation is never reached due to the process called	resonance	relaxation	saturation	none of the above			saturation
The process in which energy of the excited nucleus is transferred to another nucleus is called	the number of molecules in the	the number of molecules in	the number of molecules	none of the above			the number of molecules in the upper and lower levels become equal
The relaxation process is	relaxation	saturation	radiative transfer	non radiative transfer			relaxation
In spin-spin relaxation, the energy of the excited nucleus is transferred to	spin-spin relaxation	spin-lattice relaxation	excitation	absorption			spin-spin relaxation
The frequency of precession of the total angular momentum vector around the applied magr	stimulated	spontaneous	absorption	none of the above			spontaneous
Spin lattice relaxation is	another nucleus	electron	lattice of the crystal	none of the above			lattice of the crystal
Spin-spin relaxation is	resonance frequency	emission frequency	Larmour frequency	none of the above			Larmour frequency
NQR is a branch of ----- frequency spectroscopy which is closely related to NMR	transverse	longitudinal	parallel	none of the above			longitudinal
In NQR spectroscopy,	transverse	longitudinal	parallel	none of the above			transverse
In NQR spectroscopy, the absorption takes place in the	radio frequency	UV frequency	Microwave frequency	visible frequency			radio frequency
In NQR spectroscopy	an external magnetic field is ap	an external electric field is a	no external field is applie	external magnetic or electric field is applied			no external field is applied
In NQR, different energy levels are caused due to the interaction between	UV region	IR region	RF region	none of the above			RF region
In NQR, the energy levels are -----in nature and the transitions are ----- type	frequency of the radiation has	frequency of the radiation h	external magnetic field is	both magnetic field and frequency to be varied			frequency of the radiation has to be varied
In NMR, the energy levels are ----- in nature, and the transitions are ----- type	the nuclear quadrupole momei	the electric field gradient ar	the nuclear quadrupole n	none of the above			the nuclear quadrupole moment of the nucleus and the electric field gradient
The ESR spectrum falls in the	electrical and magnetic	magnetic and electric	electric and electric	magnetic and magnetic			electrical and magnetic
ESR is observed only in species having	electrical and magnetic	magnetic and electric	electric and electric	magnetic and magnetic			electric and electric
The magnetic moment of the electron is due to its	microwave region	rf region	UV region	IR region			microwave region
For molecules with even atomic number and mass number, has nuclear spin	paired electrons	one or more unpaired electr	nuclear quadrupole mom	none of the above			one or more unpaired electons
For molecules with odd atomic number and even mass number, the nuclear spin is	orbital motion only	spin only	both orbital motion as w	none of the above			both orbital motion as well as spin
The resonance condition in NMR is _____	half integer	integer	zero	none of the above			zero
In the relation $hv = g_N\mu_N B_{0,}$ g_N is known as ___	half integer	integer	zero	none of the above			integer
In the relation $hv = g_N\mu_N B_{0,}$ μ_N is known as ___	$hv = g_N\mu_N B_0$	$E = -\mu . B_0$	$\Delta E = 2\ \mu . B_0$	None of the above			$hv = g_N\mu_N B_0$
In both NMR and NQR absorption of radiation takes place only if _____ is achieved	Lange g factor	Nuclear g factor	Molecular g factor	None of the above			Nuclear g factor
	Bohr magneton	Magnetic moment	Nuclear magneton	None of the above			Nuclear magneton
	resonance	saturation	relaxation	none of the above			resonance

SYLLABUS

Basic principles of ESR - Experiments – ESR spectrometer reflection cavity and microwave bridge – ESR spectrum hyperfine structure - Study of free radicals – Applications of ESR
The Mossbauer effect- the recoilless emission and absorption of - Mossbauer spectrum – Experimental methods- Hyperfine interaction - Chemical Isomer Shift – Magnetic hyperfine and electric quadrupole interaction.

ESR Spectroscopy:

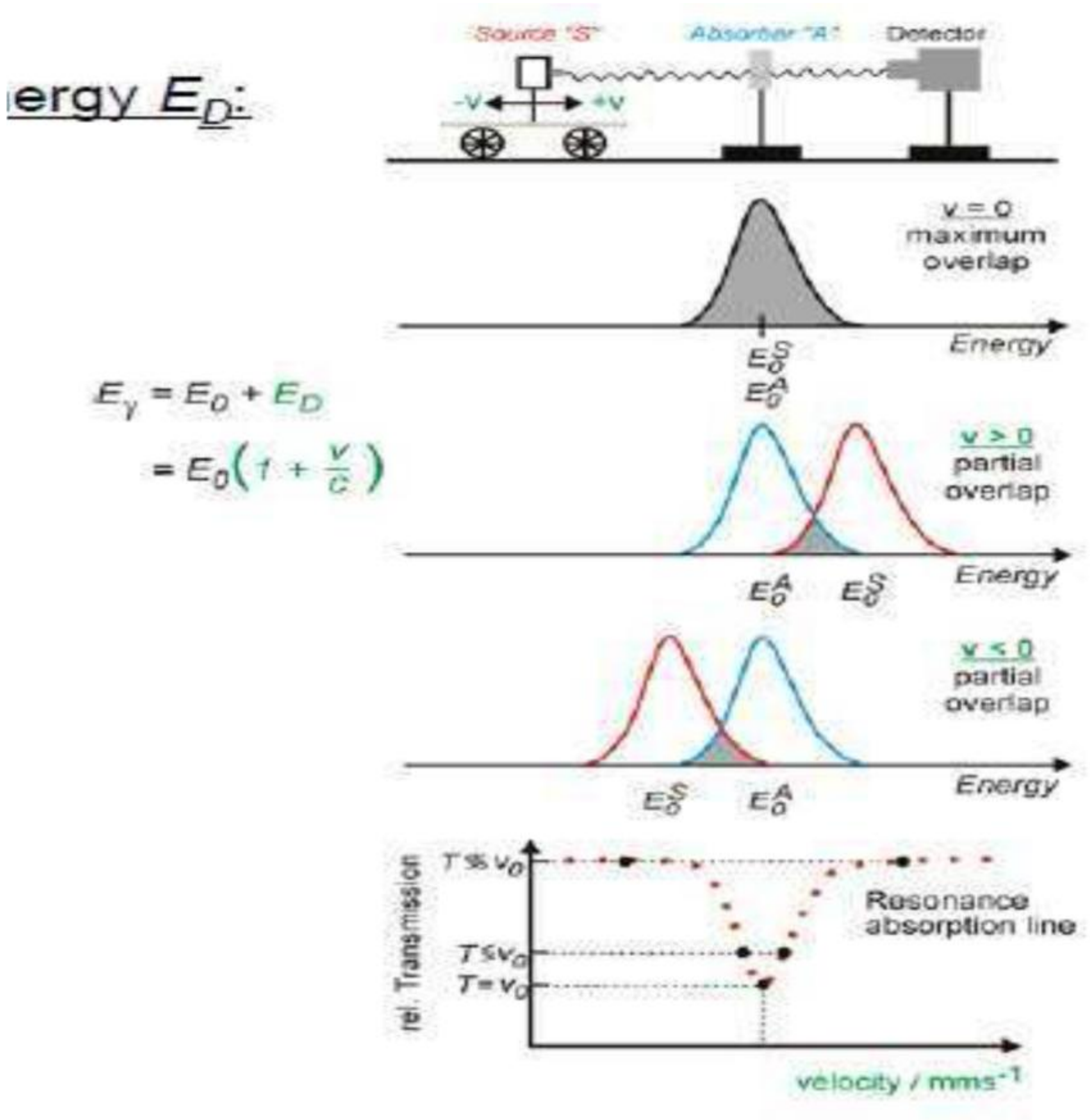
Electron Spin Resonance (ESR) spectroscopy, also referred to as Electron Paramagnetic Resonance (EPR) spectroscopy, is a versatile, nondestructive analytical technique based on the absorption of microwave radiation in presence of an applied field by paramagnetic species. When any species that contains unpaired electron(s) is subjected to a static magnetic field, the interaction between the magnetic moment of the electron and the applied magnetic field splits the spin energy levels (Zeeman splitting), and transitions between these spin levels are induced by applying suitable microwave radiation perpendicular to the magnetic field. Further interactions will depend on the presence of other factors such as the nuclear spins present in both the origin and other neigbours. The resulting absorption of the microwave radiation is modulated to record the first derivative of the absorption. Conventionally, EPR spectra are recorded as first derivative rather than absorption to improve the resolution. In fact, second derivative operation is also possible when needed to get better resolution of complex splitting patterns.

The block diagram of JES200 ESR spectrometer available at SAIF, IITM is shown below. This is a continuous wave (CW) ESR spectrometer that employs field modulation and phase sensitive detection. The Microwave Bridge consists of the Gundiode (as source of radiation) and the Detector. Both X-band (8.75 - 9.65 GHz) and Q-band (35.5GHz) frequency units are available. The sample is placed in a resonant cavity which admits microwaves through an iris. The cavity is located in the middle of an electromagnet and helps to amplify the weak signals from the sample. Other components such as an attenuator, field modulator and amplifier are also included to enhance the performance of the instrument. X- Band Electron Nuclear DOuble Resonance (ENDOR) facility is also available to study the nature of hyperfine interactions of very low magnitude, noting that this may be used only after complete understanding of the electronic structure of the molecule.

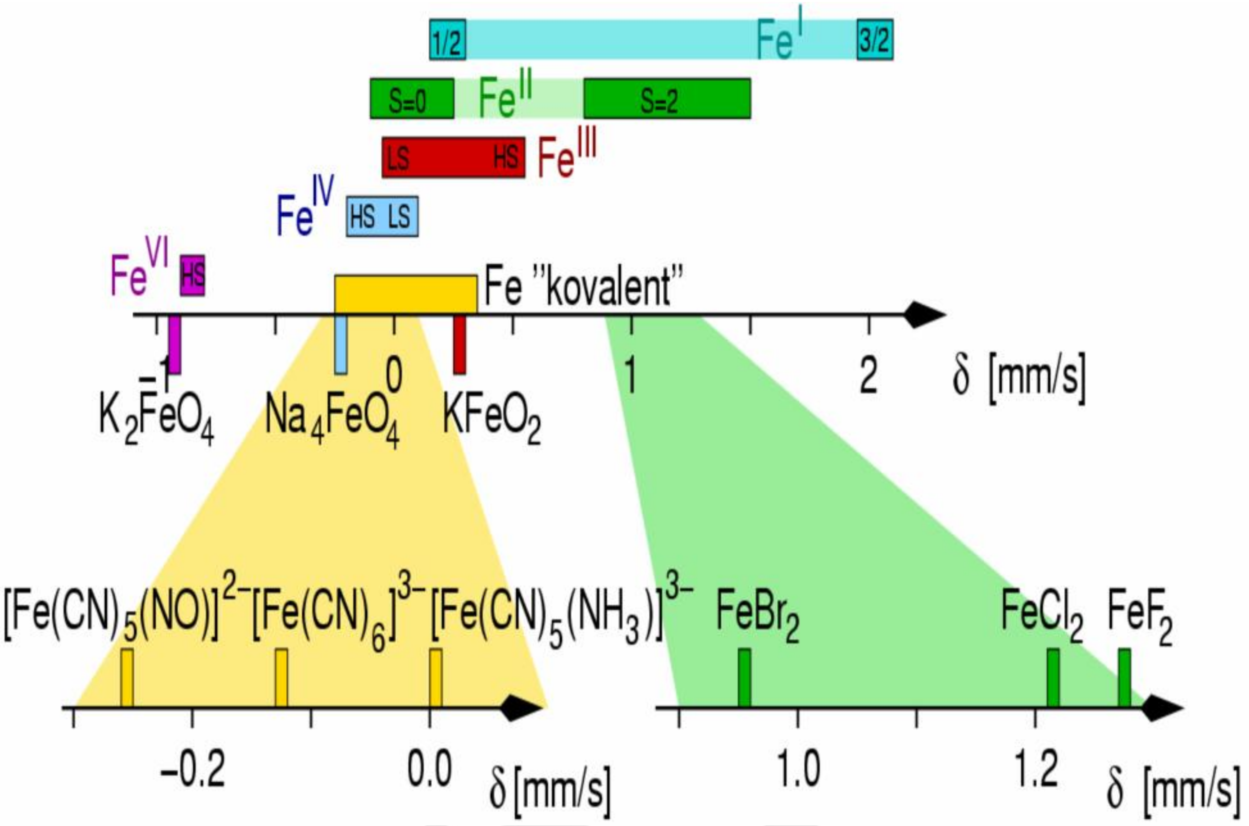
The ESR parameters that are monitored include the measurement of the g factor at the centre of the spectrum and the hyperfine splitting due to interaction with nuclei having spin $I \neq 0$. Zero-field splitting (or fine structure) characteristic of transition metal complexes and other species with two or more unpaired electrons ($S \geq 1$) can be observed in solid samples.

MOSSBAUER Spectroscopy:

Theory of Mossbauer spectroscopy:



Common samples for Mossbauer spectroscopy:

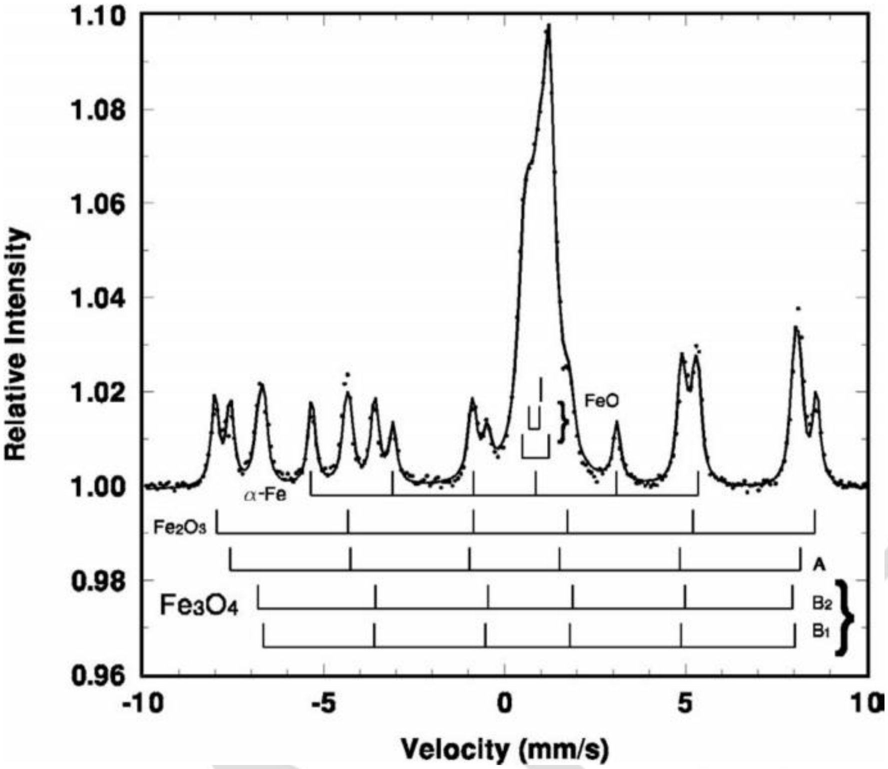


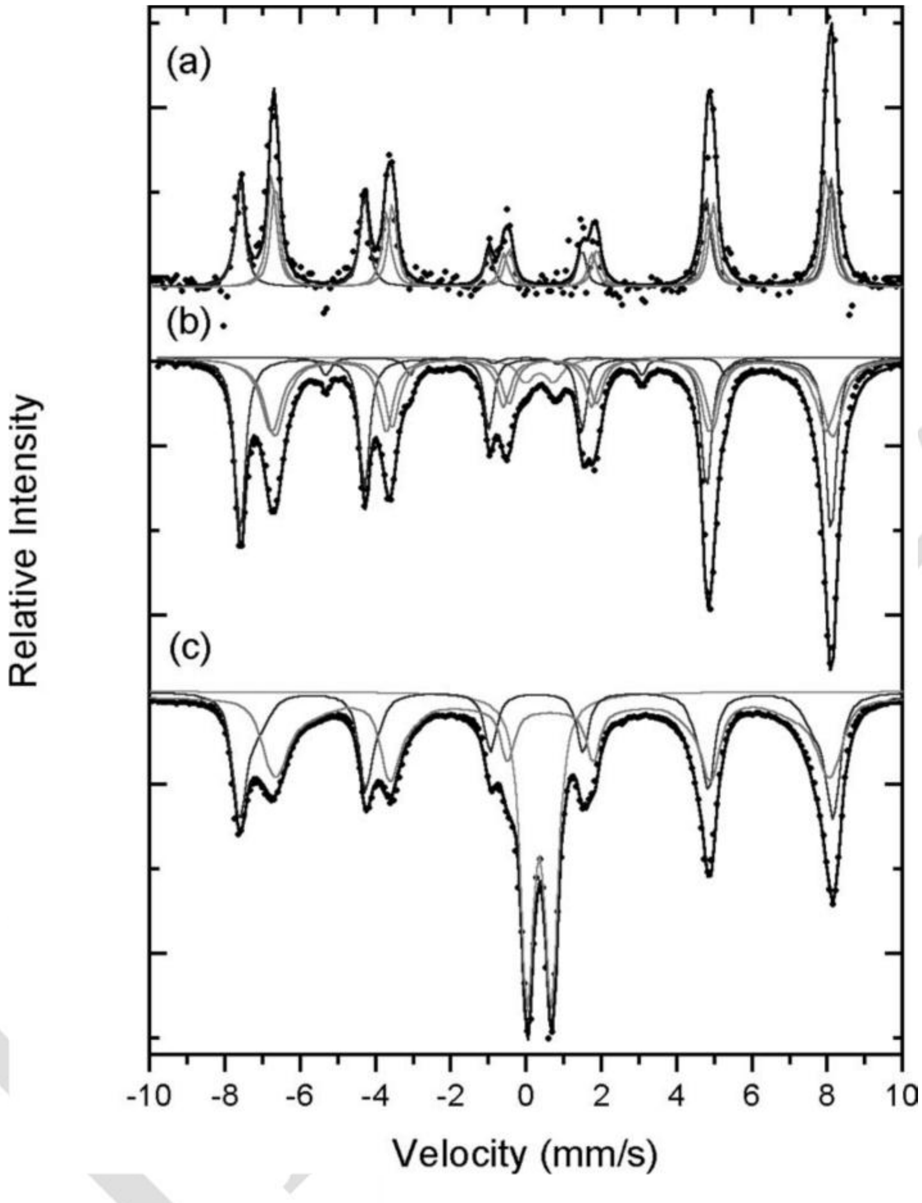
Corrosion, deterioration, and weathering of materials are age-long problems thathave faced mankind for millennia. From the world's ancient man-made and natural monoliths to today's most modern buildings, bridges and transportation facilities, the longevity of structures are closely controlled by the environments in which they are located. Having little control over these local environments, we must carefully select the materials that are best suited to the conditions to which they are exposed. Often this requires a protective coating to be applied to the material of choice. History shows however that our predecessors have often lacked the ability to predict the interaction of structures with their surroundings, and today we see deterioration of historic icons and the loss cultural relics that mark the development and achievements of humanity.

APPLICATION OF MÖSSBAUER SPECTROSCOPY:

The monitoring and evaluation of the corrosion performance of bridges and other steel structures have been extremely limited over the past 40 years. It may be considered that the serious corrosion and deterioration problems that are presently being experienced in steel and concrete bridges that are less than 25 years old, have resulted from the lack of knowledge of the performance of coated and uncoated structural steels and rebar in the adverse environments in which they are often located. Under the guidelines of the American Society for Testing and Materials, ASTM, and the International Organization for Standardization, ISO, it is common to evaluate the corrosion properties of steel, by exposing steel coupons at environmentally monitored test sites worldwide, for periods typically up to 30 years.

The test sites are classified as rural, industrial or marine according to their levels of the common airborne pollutants containing chlorides and sulfides [5]. The classification of corrosively of a test site is calculated by measuring the daily chloride and sulfide depositions as well as the time-of-wetness, which is defined as the time for which the relative humidity exceeds 80% [6]. At regular intervals, often starting at 1 year, some of the steel coupons are retrieved, the corrosion products removed, and the steel mass loss measured. Plots of mass-loss with exposure time permit the corrosion rates of the steels to be determined for their particular exposure site and its corrosivity classification.


Relative Intensity
1.10
1.08
1.06
1.04
1.02
1.00
0.98
0.96
-10
-5
0
5
10
Velocity (mm/s)
FeO
α-Fe
Fe2O3
Fe3O4
A
B2
B1



Atmospheric corrosion: protective corrosion coatings:

Structural steels can be separated into two main categories, carbon steel and alloyedsteel. Carbon steel must be used in situations where it is very well protected from exposure to both water and oxygen, and this is usually achieved by painting the clean bare surface. With time the coating will fail due to direct environmental exposure, or become porous and allow the steel beneath to corrode. For bridges, roadside guide-rails, and other large structures, this results in significant and regular repair, replacement and maintenance costs, as well as environmental problems with coating removal. If left uncoated in a normal atmospheric environment, carbon steel will corrode and the rust layer will peel from the substrate, exposing more steel to the atmosphere. The rust layer therefore offers very little protection to the carbon steel that continually loses mechanical strength and will eventually fail.

POSSIBLE QUESTIONS

1. Explain the following;
    i) Basic principles of ESR
    ii) ESR spectrum hyperfine structure
2. What is Mossbauer effect? Explain the construction and working of Mossbauer spectrometer with suitable examples.
3. Write a note on ESR spectrum hyperfine structure
4. Write a note on Applications of ESR
5. Explain the construction and working of Mossbauer spectrometer with suitable examples.
6. Write about the high resolution ESR spectroscopy and its applications.
7. What is Mossbauer effect? Explain the following
    i) Chemical Isomer Shift
    ii) Magnetic hyperfine interaction
8. Explain the construction and working of high resolution ESR spectroscopy and its applications.
9. What is ESR spectroscopy and describe about it?
10. Explain the following, Magnetic hyperfine interaction and Electric quadrupole interaction
11. A Mossbauer nucleus ^{57}Fe makes the transition from the excited state of energy 14.4 keV to the ground state. What is recoil velocity?

KARPAGAM ACADEMY OF HIGHER EDUCATION
(Under Section 3 of UGC Act 1956)
COIMBATORE – 641021
(For the candidates admitted from 2017 onwards)
DEPARTMENT OF PHYSICS
PHYSICS
SPECTROSCOPY (18PHP204)
MULTIPLE CHOICE QUESTIONS

QUESTIONS

The origin of ESR lies in the ____	**OPTION 1**	**OPTION 2**	**OPTION 3**	**OPTION 4**	**OPTION 5**	**OPTION 6**	**ANSWER**
The orientation of the magnetic dipole with respect to the applied magnetic field are							
The fact that the applied magnetic field tries to orient the magnetic moment of the electron	spin of the electron	spin of the nucleus	orbital motion of the ele	none of the above			spin of the electron
The spin of the electron can have values _____	not quantized	can be anything	quantized	in the direction of the applied field			quantized
The hyperfine structure of the ESR spectrum is due to	the magnetic moment to be ca	the magnetic moment of th	the magnetic moment to	none of the above			the magnetic moment of the electron to precess around the applied magnetic field
The mechanism by which interaction occurs due to the unpaired electron density at the nucl	+1/2 only	-1/2 only	±1/2	None of the above			±1/2
The phenomena concerned with nuclear resonant absorption and fluorescence is called	the interaction of the unpaired	interaction of the magnetic	interaction of the orbital	none of the above.			the interaction of the unpaired electron with the magnetic moments of nuclei within its orbital
The daughter nuclei in the highly excited state, produced during a radioactive decay, comes	spin-spin interaction	spin-lattice interaction	Fermi or Contact interact	None of the above			Fermi or Contact interaction
The high energy γ-ray photon emitted by a nuclear transition excites a nucleus in the ground	Mossbauer spectroscopy	ESR spectroscopy	NMR spectroscopy	NQR spectroscopy			Mossbauer spectroscopy
The recoilless absorption of the γ-ray photon is responsible for _____	visible photons	x-ray photons	γ-ray photons	none of the above			γ-ray photons
The strength of the resonant absorption is determined by the ________	absorption	the recoil energy	instrument not sensitive	none of the above			the recoil energy
The excited state of a nucleus has a mean life time of the order of ___	ESR absorption	NMR absorption	Mossbauer effect	NQR absorption			Mossbauer effect
The highest energy for which a Mossbauer effect is known is _____	overlap profile of the source ar	the peak of the absorption	the peak of the emission	none of the above.			overlap profile of the source and absorber
Mossbauer effect involves absorption of	10^{-6} s	10^{-16}s	10^{-6} ms	10^{6} s			10^{-6} s
The detector normally used to detect Mossbauer spectrum is _____	100 keV	187 keV	187 MeV	None of the above			187 keV
In Mossbauer experiment if the environment of emitting and absorbing nuclei are different,	x-rays	g-rays	UV rays	IR rays			g-rays
The Isomer shift is due to the interaction between _____	PMT	Thermocouple	Scintillator	Klystron			Scintillator
Unlike in the other branches of spectroscopy Mossbauer spectroscopy involves ____	Isotope shift	Wave length shift	Isomer shift	None of the above			Isomer shift
Splitting of Mossbauer lines are due to the interaction between _____	the nuclear charge distribution	the nuclear quadrupole mo	the nuclear magnetic mo	none of the above			the nuclear charge distribution and electron charge distribution
The isomer shift in Mossbauer spectrum is a direct function of ___	Source-absorber pair	absorber alone	source alone	other samples			Source-absorber pair
The relative movement between the source and absorber in a Mossbauer spectroscopy expe	nuclear quadrupole moment a	nuclear magnetic moment a	nuclear magnetic mome	none of the above			nuclear quadrupole moment and electric field gradient
Electron spin resonance is also known as ____	p-electron density at the nucle	s-electron density at the nu	proton density in the nuc	none of the above			s-electron density at the nucleus
The magnetic moment of the electron is due to combined effect of ___	reduction in intensity	Doppler shift	Increase in intensity	None of the above			Doppler shift
The magnetic moment of the electron is given by $\mu_s = - g\mu_B S$, where g is	nuclear magnetic resonance	electron paramagnetic reso	nuclear quadrupole reso	none of the above			electron paramagnetic resonance
The angular momentum due to spin and the magnetic moment are in ___	spin and charge	spin and mass	mass and charge	charge alone			spin and charge
For an electron since S = ½, the value of m_s is ____	Lande g factor	Nuclear g factor	Electron g factor	None of the above			Electron g factor
Spectrometers used for ESR studies in the frequency range of ~9.5 GHz are known as ____	opposite directions	same directions	perpendicular to each ot	any orientation			opposite directions
Q band spectrometers are operated at frequencies of the order of ____	½	- ½	± ½	1			± ½
The hyperfine Structure of ESR spectrum is due to ___	Q-band spectrometers	X-band spectrometers	S-band spectrometers	None of the above			X-band spectrometers
ESR involves ________	~9.5 GHz	~35 GHz	~9.5 MHz	~35 MHz			~35 GHz
	nuclear spin	electron spin	dipole-dipole interaction	none of the above			dipole-dipole interaction
	absorption	emission	scattering	radiation			absorption