Chhatrapati Shahu Ji Maharaj University, Kanpur

Answer Script Details
Barcode 10877268

Roll No. 24063001034
Total Mark 49/75.00

Exam MASTER OF SCIENCE _ODD EXAM-DEC-24
Subject B020704T - SPECTROSCOPY

Question wise Mark Summary

Q.No	Mark	Q.No	Mark	Q.No	Mark	Q.No	Mark
1A	4/5	6A	NA/7				
1B	4/5	6B	NA/7				
1C	4/5	7A	NA/7				
1D	NA/5	7B	NA/7				
1E	4/5	8A	5/7				
1F	3/5	8B	6/7				
1G	4/5	9A	NA/7				
1H	4/5	9B	NA/7				
1I	NA/5						
2A	6/7						
2B	5/7						
3A	NA/7						
3B	NA/7						
4A	NA/7						
4B	NA/7						
5A	NA/7						
5B	NA/7						

PART-I

Date of Exam : 30/1/25 Shift : 1st Room No.: 20

Paper Code: B020704T Subject: Spectroscopy Year/Sem: 1st

Name of Candidate: Priya Kumari Gupta

Roll No. 2 4 0 6 3 0 0 1 0 3 4

COE Facsimile

Signature of Invigilator

Priya Kumari Gupta
Signature of Candidate

Chhatrapati Shahu Ji Maharaj University
Kanpur, Uttar Pradesh

PART-II

MARKS OBTAINED

Q.	1	2	3	4	5	6	7	8	9	10
(a)										
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(c)										
(d)										
(e)										
(f)										
(g)										
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(i)										
(j)										
Total										

Total Marks in Figures ______ Max. Marks

Total Marks in Words

B 0 2 0 7 0 4 T
Paper Code

Signature of Evaluator

PART-III

Course MSCCH (Chemistry)

Session 2024-25 Year/Semester 1st

Subject Spectroscopy

Paper Code

B 0 2 0 7 0 4 T

Exam Date

3 0 - 1 - 2 5

Name of Candidate

P R I Y A K U M A R I
G U P T A

Father's Name

S A M B H U N A T H
P R A S A D

महाविद्यालय का कोड
College Code

U	N	0	1	
Ⓐ	Ⓐ	●	⓪	⓪
Ⓔ	Ⓑ	①	●	①
Ⓕ	Ⓓ	②	②	②
Ⓗ	Ⓙ	③	③	③
Ⓚ	Ⓚ	④	④	④
Ⓛ	Ⓛ	⑤	⑤	⑤
Ⓡ	Ⓜ	⑥	⑥	⑥
Ⓢ	●	⑦	⑦	⑦
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परीक्षा केन्द्र का कोड
Exam Centre Code

U	N	0	1	
Ⓐ	Ⓐ	●	⓪	⓪
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परीक्षा का प्रकार
Type of Exam

संस्थागत Regular ● भूतपूर्व छात्र Ex. Student ○

व्यक्तिगत Private ○ बैक पेपर परीक्षा Back paper Exam ○

ANSWER BOOKLET NO.

10877268

B 0 2 0 7 0 4 T
Paper Code

नामांकन संख्या
Enrollment Number C S J M A 2 4 0 0 0 0 6 3 1 7 1

परीक्षार्थी अनुक्रमांक संख्या Candidate's Roll Number

2	4	0	6	3	0	0	1	0	3	4
⓪	⓪	●	⓪	⓪	●	●	⓪	●	⓪	⓪
①	①	①	①	①	①	①	●	①	①	①
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④	●	④	④	④	④	④	④	④	④	●
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⑥	⑥	⑥	●	⑥	⑥	⑥	⑥	⑥	⑥	⑥
⑦	⑦	⑦	⑦	⑦	⑦	⑦	⑦	⑦	⑦	⑦
⑧	⑧	⑧	⑧	⑧	⑧	⑧	⑧	⑧	⑧	⑧
⑨	⑨	⑨	⑨	⑨	⑨	⑨	⑨	⑨	⑨	⑨

पेपर कोड Paper Code

B	0	2	0	7	0	4	T
Ⓐ	●	⓪	●	⓪	●	⓪	Ⓝ
●	①	①	①	①	①	①	Ⓟ
Ⓒ	②	●	②	②	②	②	Ⓡ
Ⓔ	③	③	③	③	③	③	●
Ⓕ	④	④	④	④	④	●	
Ⓖ	⑤	⑤	⑤	⑤	⑤	⑤	
Ⓩ	⑥	⑥	⑥	⑥	⑥	⑥	
[illegible]	⑦	⑦	⑦	●	⑦	⑦	
[illegible]	⑧	⑧	⑧	⑧	⑧	⑧	
	⑨	⑨	⑨	⑨	⑨	⑨	

Priya Kumari Gupta
Signature of Candidate

Signature of Invigilator

C S Facsimile

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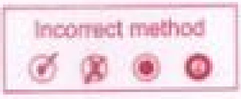
नोट : 1. परीक्षार्थी को निर्देशित किया जाता है कि आवरण पन्ने के पृष्ठ भाग पर अंकित सभी निर्देशों को सावधानी पूर्वक पढ़ें।
2. बॉक्स में भरी जाने वाली प्रविष्टियाँ बायीं तरफ से शुरू की जायें। 3. गोलों को काले या नीले बॉलपेन से भरा जायें।

INSTRUCTIONS TO THE CANDIDATE FOR FILLING PART-I

1. Read the instructions carefully given on the answer script and admit card.
2. Write Date of Exam, Shift, Paper Code & Name of Subject Correctly.
3. Write Name & Roll No. Correctly.
4. Write Semester & Branch Correctly.

INSTRUCTIONS TO THE CANDIDATE FOR FILLING PART-III

1. Use blue or black ball point pen for writing alphabets & numerals in ☐ Boxes.
2. Carefully study the example before you start marking.
3. As shown in the example below blacken the circles completely.



4. Make no Stray marks on this sheet.
5. **DO NOT WRITE OR MARK ON THE BAR CODE.**

IN ORDER TO AVOID UFM (UNFAIR MEANS) :

1. The Roll No. and Answer Book no. found elsewhere or any other symbol found in the answer book will be treated as unfair means.
2. Any tempering of Bar Code and Booklet no shall be treated as Unfair Means.
3. Do Not bring the materials like slip of paper/mobile/digital diaries/ study material/ revision notes in examination hall. Possession of the mobiles/ digital diaries/ electronic watch and any other electronic gadget except memory less scientific calculator shall be considered as UFM case.
4. Do not keep or paste currency note in answer script it shall be consider as UFM.

अनुचित साधन से बचने हेतु:

1. उत्तर पुस्तिका के निर्देशित स्थान को छोड़कर अनुक्रमांक एवं उत्तरपुस्तिका का क्रमांक कहीं और न लिखे तथा कोई भी चिन्ह न बनावें क्योंकि यह अनुचित साधन प्रयोग की परिधि में आता है।
2. उत्तर पुस्तिका के बारकोड अथवा उत्तर पुस्तिका संख्या पर छेड़ करने पर अनुचित साधन प्रयोग माना जायेगा।
3. परीक्षा कक्ष में निम्न वस्तुएं साथ न लावें, जैसे लिखे हुए कागज के टुकड़े, मोबाईल, डिजिटल डायरी, कॉपी, पुस्तक यह सभी वस्तुएं जो अनुचित साधन के अन्तर्गत आती है। केवल संबंधित प्रश्नपत्र में ही मेमोरी लैस साइंटफिक कैल्कुलेटर ले जाने की अनुमन्यता होगी।
4. उत्तर पुस्तिकाओं में रूपये न रखें न ही उत्तर पुस्तिका में चिपकायें। ऐसा करना अनुचित साधन प्रयोग की परिधि में आता है।

परीक्षार्थी के लिए निर्देश

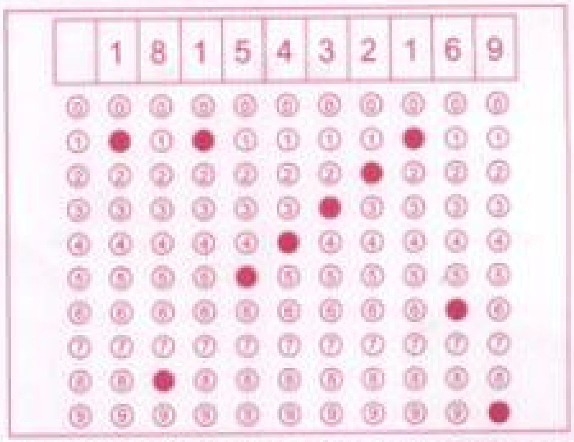
1. प्रवेश पत्र एवं उत्तर पुस्तिका पर दिये गये निर्देशों को ध्यान से पढ़ें।
2. कवर पृष्ठ के दूसरी तरफ कुछ न लिखें।
3. उत्तर पुस्तिका के पृष्ठों पर दोनों तरफ लिखें।
4. प्रश्न पत्र पर अपने अनुक्रमांक के अतिरिक्त कुछ न लिखें।
5. प्रश्न पत्र कोड एवं प्रश्न पत्र कोड सावधानी पूर्वक लिखें।
6. अपनी स्थिति स्पष्ट लिखें।
7. उत्तर पुस्तिका के पृष्ठों की संख्या देखें। अगर उत्तर पुस्तिका में पृष् (1–24) से कम है या फटे हुए है, तो परीक्षा शुरू होने के पूर्व दूसरी उत्त पुस्तिका ले लें।
8. प्रश्नपत्र को देखे, यदि प्रश्नपत्र के विषय कोड, विषय का नाम तथा प्रश्न में कोई त्रुटि है तो उसके परीक्षा शुरू होने के 30 मिनट के अन्दर कक निरीक्षक को तत्काल सूचित करें, उसके बाद विश्वविद्यालय द्वारा को कार्यवाही नहीं की जायेगी।
9. प्रश्नों के उत्तर लिखने के लिये पैंसिल का प्रयोग न करें।
10. B कॉपी या अतिरिक्त ग्राफ नहीं दिया जायेगा।

INSTRUCTIONS TO THE CANDIDATE

1. Read the instructions carefully given on the Question Pape Admit Card & Answer Script.
2. Do not write anything on back side of the cover page.
3. Write on both sides of pages of answer book.
4. Do not write anything on question paper except Roll Number.
5. Write Paper Code & Question Paper Id carefully.
6. CHECK the number of pages (1-32) or any other kind of damag in your answer script, if found than change the answer scrip immediately before the commencement of examination.
7. CHECK the Question Paper for any kind of discrepancy e. Subject Code, Subject Name and Question of the Questio Paper during first THIRTY MINUTES of the commencement the exam, so that it can be corrected in TIME. After that n corrections shall be entertained by the university.
8. Do not use pencil for answering the question.
9. Write status correctly e.g. those appearihg in carry over pape should fill in status as Carry Over. Those appearing as E Students should fill in status as ex.
10. No supplementary answer book & graph paper will be provided.

INSTRUCTIONS TO THE CANDIDATE FOR FILLING PART-IV

1. Use blue or black ball point pen for writing alphabets & numerals in ☐ Boxes.
2. Use blue or black ball point pen for filling the circles.



Note - If your Roll No. is of 10 digits. Please leave first three colum

Paper Code

Section-C

8.a)

Nuclear Quadrupole Resonance (NQR) is a spectroscopic technique that detects the interaction between the electric quadrupole moment of [illegible] nucleus and the electric field gradient in a material.

The basic principles of NQR are as follows:-

- Certain nuclei e.g. N, Cl, Cu have a non-spherical charge distribution, leading to a quadrupole moment.

- This moment interacts with the surrounding EFG produced by non-symmetric charge distributions in molecules.

Energy level splitting -

- In presence of an EFG, the quadrupole nucleus experiences an interaction that splits nuclear energy levels.
- The number and pattern of energy levels depend on the nuclear spin I.

For $I = 1$ → Two energy levels.
For $I = 3/2, 2, 5/2$, etc - Multiple energy levels.

Resonance condition -

When the nucleus is exposed to radiofrequency (RF) radiation matching the energy difference between levels, resonance absorption occurs.

b) Nuclei with spin ≥ 1, such as N^{14}, Cl^{35}, Cu^{65} have an electric quadrupole moment so that their energy split by electric field gradient due to electronic bonds [illegible] the chemical environment is called ~~nuet~~ quadrupole nuclei.

Since, the quadrupole ~~nuclear~~ moment arises from an unsymmetrical distribution of electric charge in the nucleus, it is an electric moment rather than magnetic moment.

• If the nucleus is spherical ($I = 0$ or $\frac{1}{2}$) or if the electron environment around the nucleus is spherical all the nuclear orientation are equivalent and the corresponding quadrupole energies are degenerate

• The energy difference between various levels and hence, the frequency of transition will depend upon the field gradient produced by valence electron and the quadrupole moment of the nucleus.

The quadrupole moment Q, is the measure of deviation of the electric charge distribution of the nucleus from spherical symmetry.

The quadrupole moment can be expressed in term of nuclear dimensions by relation:-

$$Q = \frac{1}{e}\int \rho_0^2 (3\cos^2\theta - 1)\, d\tau = \tau(3z^2 - r^2)A.$$

where $e >$ fundamental charge

$\rho >$ nuclear charge

r = distance from centre of gravity.
θ = angle between z and spin axis.

Q=0

Q<0 (oblate)

Q>0 (prolate).

- If positive value of Q indicates that the nucleus is prolate.
- The negative value of Q indicates that the nucleus is prolate

- Splitting of energy is given by:

$$E_m = \frac{e^2Qq\,[3M_I^2 - I(I+1)]}{4I(2I-1)}$$

I = nuclear spin quantum number.
M_I = nuclear quadrupole moment.
e^2Qq = nuclear coupling ~~central~~ constant.

e.g. $_7N^{14}$ (nuclear spin $I=1$)

$M_I = -1, 0, +1$ but $M_I = \pm 1$ are degenerate.

$$E = \frac{e^2Qq\,[3\times \text{[illegible]}\,1(1+1)]}{4\times1(2\times1-1)}$$

$$E = \frac{e^2Qq}{4}.$$

Section - B.

2. a) Raman effect is easily understable on the basis of quantum theory of radiation. This theory shows that the problem of intensities of Raman lines and prediction of selection rule.
Correctly whereas the classical theory of could not show this problem.

According to quantum theory, Raman effect is considered to be the outcome of the collision between the light photons and molecule. Thus applying the principle of conservation of energy

$$E_p + \frac{1}{2}mv^2 + h\nu_i{}^2 = E_q + \frac{1}{2}mv'^2 + h\nu_s \ldots$$

where,
E_p and E_q are the intrinsic energies before and after collision
v and v' are the velocities of the molecule before and after collision
ν_i and ν_s are the frequency of the incident and scattered photons respectively.

As the collision does not change cause any appreciable change of temperature it may be assumed that the kinetic energy of the molecule remains practically unchanged in the process.

$$E_p + h\nu_i = E_q + h\nu_s$$

$$h(\nu_s - \nu_i) = E_p - E_q$$

$$\nu_s = \nu_i + \frac{E_p - E_q}{h}$$

There are 3 possibilities which arises due to :-

i) If $E_p = E_q$ then $\nu_s = \nu_i$ which represent unmodified lines called Rayleigh lines.

ii) If $E_p > E_q$ then $\nu_s > \nu_i$ which represents anti-strokes lines.

iii) If $E_p < E_q$ then $\nu_s < \nu_i$ which represents strokes line.

b) Strokes Lines:-

- These appear when the scattered photon has less energy than the incident photon.
- This happens because the molecules absorbe some energy from the photon, transitioning to a higher vibrational state.
- Strokes lines are more intence than anti-strokes lines because most molecules are initially in the ground state at room temperature.

Anti- Stokes ~~like~~ lines:-

These appear when the scattered photon has more energy than the incident photon.

- This occurs when the molecule is already in an excited vibrational state and then loses energy to the scattered photon, returning to a lower state.

- Since fewer molecules start in a excited state anti-stroke lines are typically weaker than Stokes lines.

Significance in spectroscopy :-

- Temperature dependence – The intensity ratio of stokes to anti- stoke lines provide information about the temperature of the sample.

- Material identification – The shift in frequency of these lines helps in determining molecular structures and composition.

Sec-A.

1. a) Spectroscopy is the scientific study of the interaction between matter and electromagnetic radiation. Different types of spectroscopy are IR, UV, visible, x-ray, etc are used for various application. Each atoms and molecules has a unique spectra. As a result these spectra can be used to detect, identify and quantify information about the atoms and molecules.

Electromagnetic Radiation is a form of energy that is transmitted through space as waves or particles. It consist of oscillating electric and magnetic field that are perpendicular to each other and to the direction of propagation. These waves travels at the speed of light in a vacuum and do not need a medium for transition. EMR encompasses a wide range of wavelength and frequency collision known as spectrum.

Gamma > X-Rays < UV < visible < IR < Microwave < Radio.

	λ	Source
Gamma	$< 10^{-12}$m	Nuclear radiation, radioactive decay.
x-ray	$10^{-12} - 10^{-8}$m	accelerated electron
UV	$10^{-8} - 10^{-7}$m	Sunlight
visible	380 - 750nm	Sunlight, laser.
IR	$10^{-6} - 10^{-3}$m	heat emitting object
Microwave	$10^{-3} - 10^{-1}$m	Radar, satellite
Radio wave	$> 10^{-1}$m	GPS, telecommunication

b) The selection rule of Raman spectroscopy is based on the polarizability ~~of~~ the molecules. It states that :-

"For a molecula[illegible]ration to be Raman active, it must cause a change in the polarizability of the molecule".

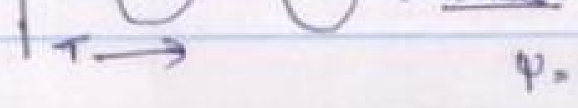
Polarizability Change – The vibration must lead to a fluctuation in the energy of the molecules in which the molecule should have free energy in the vibration.

+ Concentration of species – The species having higher concentration will lead to greater splitting in the spectral lines.

The selection Rule states that $\Delta S = \pm 1$.
If $\Delta S = 1$, it represents the Strokes lines.
If $\Delta S = -1$, it represents anti-strokes lines.

d) The oscillation of a molecule in single 1-dimensional box in x or y or z axis is said to simple harmonic oscillator.
The wave functi[illegible]f simple harmonic oscillation is given by , $\psi = A \sin \frac{2\pi x}{\lambda}$

The atom or molecule oscillate in single orientation. This orientation leads to simple harmonic motion.



$\psi = A \sin \frac{2\pi x}{\lambda}$

i) a) The splitting of spectral line in more than one cent column in presence of electric field is said to be Stark effect.

- Stark effect is caused due to spin orientation of the molecule. It leads to splitting of spectral lines due to its orientation. The orientation in the molecule is along the axis of field effect.

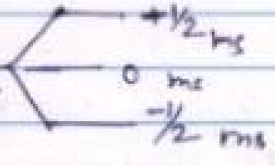
- Stark effect is due to inter-ionic or dipole-dipole interaction among the molecules and the electronic spin

- The splitting of the energy levels are are represented by formula $(2l+1)$. The splitting is shown by following diagram.

- If $l=1$, It represent the splitting as :-

$(2\times1+1) = 3$. this is $+1, 0, -1$ or we can say say no spin axis in $+1/2, 0, -1/2$.

Fig.



} splitting of spectrum in 3 lines.

n-axis

This splitting presence of presence of electric field is said to be Stark effect.

8) Nuclear magnetic Resonance (NMR) is a technique used to identify the structure of molecule and the chemical environment around the nucleus. The nucleus is surrounded by negatively charged electrons where the nucleus is positively changed. This technique is used to identify the structure as well as the composition of [illegible] and its surrounding environment.

Few limitations of NMR spectroscopy are as follows

- It uses a large quantity of sample i.e. 0.5ml of sample whose concentration is 1% of the solution.

- NMR Spectroscopy is very speed restrictive. It completes the reaction within fraction of seconds. i.e. 10-15 microseconds.

- It cannot detect the ~~same~~ different hydrogen atoms of the same compound. It shows the resonance spectrum in the overlapped form.

- While detecting [illegible] compound, it detects only molecular wei[illegible] does not talks about molecular composition, its [illegible]tting in changed solvent, etc.

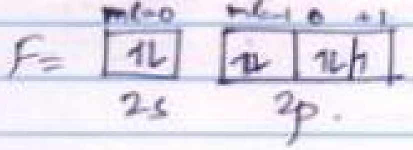
The reason for using Tetramethyl Silance (TMS) in NMR spectroscopy are the above reasons:

- Within a small quantity of sample it can detect the nucleus of the sample.
- It is speed sensitive.

a) Mutual exculsion principle states that no two electrons with same spin can occupy the orbital with same energy. The spin of the electron should be different for the electron to occupy the single orbital.
The spin of the electrons are represented by $+\frac{1}{2}$ or $-\frac{1}{2}$ or by a symbol ↑ or ↓.

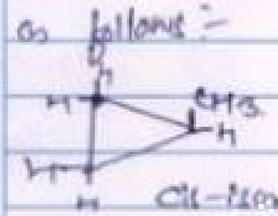
For. eg. Let us consider the example of F atom. The electronic configuration of F atom is – $1s^2 2s^2 2p^5$.

$F = 1s^2\, 2s^2\, 2p^5$

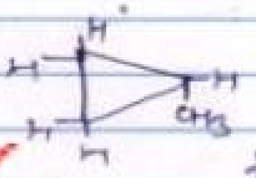


The above orbital diagram shows that 2s orbital is having 2 electrons and each electron is having the spin opposite to each other. The spins are opposite to avoid inter-electronic repulsion among the electrons in the same orbital.

b) The cis- and trans isomers of methylcyclopropane are as follows :-



cis-isomer



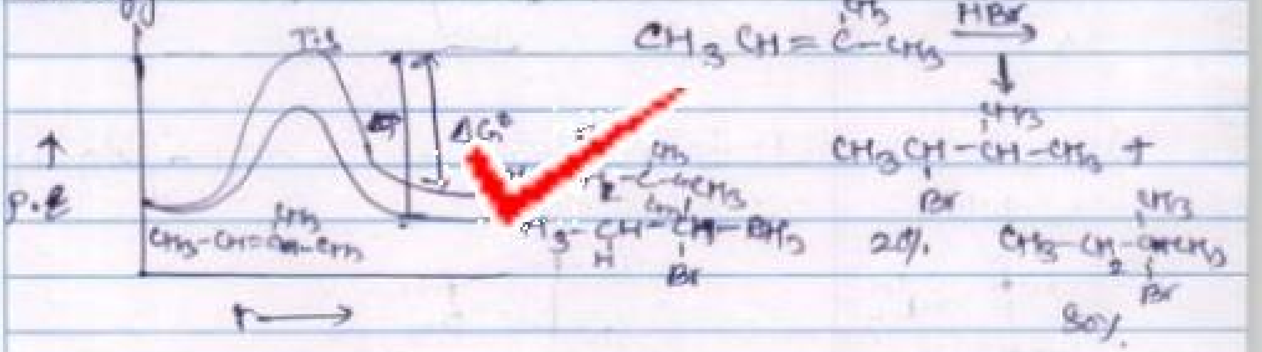
trans-isomer

When PMR radiation is passed through a sample of isomers of ~~cyclo~~ methylcyclopropane then the radiation causes vibration of particles in its axis of rotation.

The cis-methylcyclopropane ~~shows~~ does not show the deflection in magnetic field. ~~It~~ It is due to orientation of the molecule in the direction of magnetic field.
The molecules vibrate in the mean position without causing any spectral splitting.

The trans-methylcyclopropane shows the deflection in magnetic field. It is due to the orientation of the molecule in ~~the~~ in the direction perpendicular to the direction of magnetic field.
The molecules vibrate and oscillate in the mean position as well as in the direction perpendicular to magnetic field lines causes the splitting of spectral lines in more directions compared to cis-isomer.

e) On ~~[illegible]~~ potential energy diagram the difference in energy gaps between the two isomers of single from ground state to transition state is called zero point energy.



$CH_3CH=\overset{CH_3}{C}-CH_3 \xrightarrow{HBr}$

$CH_3\underset{Br}{CH}-\overset{CH_3}{CH}-CH_3$ + 20%

$CH_3-CH_2-\overset{CH_3}{\underset{Br}{C}}-CH_3$ 80%

The energy gap between the transition state of 2 molecular compounds leads to zero point energy.

15 It states that electronic transition occur so rapidly compared to nuclear motion that the nuclei of the molecule remain essentially fixed during the transition.
This is due to large difference in mass between electron and nuclei.

- Vertical Transition - Because nuclei do not move significantly during an electronic transition, the transition is best represented by vertical transition.

- Vibrational overlap - The intensity of electronic transition depends on the overlap between the vibrational wave functions of the initial and final states.

- Stokes shift - In fluorescence light, the emitted light is usually of lower energy than the absorbed light due to vibrational relaxation in the excited state.

This theory is used to explain absorption and emission spectra, fluorescence, phosphorescence and Raman spectroscopy.

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