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C.B.S. (6th Semester)
EXAMINATION, May - June, 2022
ATOMIC AND MOLECULAR
SPECTROSCOPY
(C-601)

Time : Three Hours]

[Maximum Marks:40

Note: Attempt all sections as directed.**(Section-A)****(½ mark each)****(Objective/Multiple Choice Questions)****Note: Attempt all questions:**

1. Which set of transition is correct?

- (A) $\sigma - \sigma^* < \pi - \pi^*$
 (B) $\sigma - \sigma^* > \pi - \pi^*$
 (C) $\sigma - \sigma^* = \pi - \pi^*$
 (D) None

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2. Coarse and fine structure are produced by :

- (A) Through electronic transition
 (B) Vibrational and rotational energy changes
 (C) Rotational and translational energy changes
 (D) Translational and vibrational energy changes

3. According to Born Oppenheimer approximation the total energy of a molecule in the ground state is given by

- (A) $E_{\text{total}} = E_{\text{R}} + E_{\text{V}} + E_{\text{e}}$
 (B) $E_{\text{total}} = E_{\text{T}} + E_{\text{R}} + E_{\text{V}} + E_{\text{e}} + E_{\text{n}}$
 (C) $E_{\text{total}} = E_{\text{R}} + E_{\text{V}} + E_{\text{e}}$
 (D) None of these

4. "An electronic transition takes place so rapidly that a vibrating molecule does not change its internuclear distance appreciably during the transition", this is given by:

- (A) Born-Oppenheimer
 (B) Lambert and Beer
 (C) Franck and Condon
 (D) Stark-Einstein

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5. Among the following which is rotational active in microwave region:

(A) N_2

(B) O_2

(C) HCl

(D) Cl_2

6. Identify correct selection rule for the transition between the rotational energy level:

(A) $\Delta J = \pm 1$

(B) $\Delta J = \pm 2$

(C) $\Delta J = \pm 3$

(D) $\Delta J = \pm 0$

7. Calculate the degeneracy of 3rd excited state of rotational level?

(A) 7

(B) 8

(C) 9

(D) 10

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8. The spectroscopic technique that can distinguish unambiguously between trans-1, 2, dichloroethylene and cis-1, 2 dichloroethylene without any numerical calculation is :

(A) Microwave spectroscopy

(B) UV-Visible spectroscopy

(C) X-ray photoelectron spectroscopy

(D) Gamma-ray spectroscopy

9. The selection rule of the P, Q and R-branches, respectively are

(A) $\Delta V = +1, \Delta J = -1$; $\Delta V = +1, \Delta J = 0$; $\Delta V = +1, \Delta J = +1$

(B) $\Delta V = -1, \Delta J = -1$; $\Delta V = +1, \Delta J = 0$; $\Delta V = -1, \Delta J = -1$

(C) $\Delta V = +1, \Delta J = +1$; $\Delta V = +1, \Delta J = +1$; $\Delta V = +1, \Delta J = +1$

(D) $\Delta V = -1, \Delta J = -1$; $\Delta V = +1, \Delta J = -1$; $\Delta V = -1, \Delta J = -1$

10. Intense band generally observed for a carbonyl group in the IR spectrum is due to

(A) The force constant of CO bond is large

(B) The force constant of CO bond is small

(C) There is no change in dipole moment for CO bond stretching

(D) The dipole moment change due to CO bond stretching is large

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11. How many vibrational modes are present in CO_2
- (A) 2
 - (B) 3
 - (C) 4
 - (D) 1
12. IR spectra observed in the
- (A) Gaseous state
 - (B) Liquid state
 - (C) Solid state
 - (D) All of these
13. The most commonly used laser for Raman Spectroscopy is
- (A) ND:YAG
 - (B) Ruby laser
 - (C) He-Ne laser
 - (D) Semiconductor Laser
14. The Raman spectrum is said to consist of Stokes lines when _____
- (A) $\Delta\nu > 0$
 - (B) $\Delta\nu < 0$
 - (C) $\Delta\nu = 0$
 - (D) Does not depend on $\Delta\nu$

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15. Which of the following lines are most intense?
- (A) Stokes lines
 - (B) Rayleigh Scattering lines
 - (C) Anti-Stokes lines
 - (D) All have same intensity
16. Which of the following cannot be conserved during Raman scattering?
- (A) Total Energy
 - (B) Momentum
 - (C) Kinetic Energy
 - (D) Electronic Energy
17. Predict the number of lines in ESR spectra of the following systems respectively
- a. CH_3CH_2 2. CH_3 3. C_6H_6
- (A) 4, 7, 6
 - (B) 2, 1, 6
 - (C) 5, 3, 6
 - (D) 12, 4, 7

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18. Which of the following will not show ESR spectra

- (A) O_2
- (B) C_2H_5
- (C) N_2
- (D) Cu^{2+}

19. An increase in conjugation is correlated with ---- in the energy of the LUMO, --- in the energy of the HOMO, and --- in λ_{max}

- (A) A decrease, an increase, a decrease
- (B) A decrease, an increase, an increase
- (C) An increase, a decrease, a decrease
- (D) An increase, a decrease, an decrease

20. 2.5×10^{-4} M solution of substance in 1 cm length cell at $\lambda_{max} = 245$ nm has absorbance 1.17 cm, calculate ϵ_{max} for this transition-

- (A) $0.468 \times 10^{-7} \text{ cm}^2 \text{ mol}^{-1}$
- (B) $4.68 \times 10^{-7} \text{ cm}^2 \text{ mol}^{-1}$
- (C) $0.468 \times 10^7 \text{ cm}^2 \text{ mol}^{-1}$
- (D) $4.68 \times 10^7 \text{ cm}^2 \text{ mol}^{-1}$

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(Section-B)

(Very Short Answer Type Questions)

(0.75 marks each)

Note: Attempt all questions:

1. Give briefly various regions of electromagnetic radiation or spectrum.
2. The possible electronic transition for CH_3Cl molecule
3. What is starck effect?
4. _____ top molecules has three rotational constant.
5. The vibrational frequency and anhormonycity constant of a molecule are 300 cm^{-1} and 0.0025 respectively calculate bond dissociation energy.
6. What is the basis condition for IR active molecule?
7. The Raman shift generally lies between.
8. Write the selection rule for rotational vibrational Raman spectra.
9. What is the effect of solvent on electronic spectra?
10. What is superfine splitting?

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(Section-C)

(Short Answer Type Questions)

(1.25 marks each)

Note: Attempt all questions:

1. What do you mean by B-O approximation? Explain with example.
2. Write about Maxwell Boltzmann distribution.
3. Classify molecule according to rotational spectroscopy.
4. Find the transition energy in terms of B when transition takes place from 3rd excited state to 4th excited state.
5. Write a note on isotopic effect on rotational spectra.
6. What do you mean by Fermi resonance? Explain with example.
7. Give the formula for calculating the Raman shift ($\Delta\nu$).
8. What is mutual exclusion principle?
9. What is hyperfine splitting in ESR spectroscopy? Explain with spectra of CH₃ radical.
10. Write a note on molecular photoelectron spectroscopy.

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(Section-D)

(Short Answer Type Questions)

(2 marks each)

Note: Attempt all questions:

1. Describe all type of electronic transition.

OR

Give the qualitative description of Frank-condon principle.

2. In rotational spectra of CO gas the spacing between rotational line is 3.844 cm⁻¹.

OR

Describe rotational spectroscopy of rigid diatomic molecules.

3. The fundamental and hot band of CO molecule appears at 2143.1 cm⁻¹ and 2116.1 cm⁻¹ respectively. Calculate the position of 1st overtone.

OR

The position of 1st P-branch and 1st R-branch of HCl molecule appears at 2865.1 cm⁻¹ and 2906.24 cm⁻¹ respectively. If the temperature of the sample is 300 K then calculate the value of rotational constant in cm⁻¹.

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4. Write the application of Raman Spectroscopy.

OR

What is Raman spectrum? What is essential criteria for a molecule to be Raman active?

5. Explain the instrumentation of electronic spectroscopy.

OR

What is the Tensor quantity? How can you determine the tensor-g quantity?