

BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

CLASS: MSC./IMSC/PRE-PHD
BRANCH: CHEMISTRY

SEMESTER : III/ IX/I
SESSION : MO/2025

SUBJECT: CH503 MOLECULAR SPECTROSCOPY

TIME: 3 HOURS

FULL MARKS: 50

INSTRUCTIONS:

1. The question paper contains 5 questions each of 10 marks and total 50 marks.
 2. Attempt all questions.
 3. The missing data, if any, may be assumed suitably.
 4. Before attempting the question paper, be sure that you have got the correct question paper.
 5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.
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| Q.1(a) Write down the rotational kets of a symmetric top molecule with J=2. Arrange them in the order of increasing energy. | [5] 1 | 2 |
| Q.1(b) Explain the origin of the alternation in intensity in the rotational Raman spectrum of $^1\text{H}_2$. | [5] 1 | 3 |
| Q.2(a) Derive the gross and specific selection rules in vibrational spectroscopy. Assume the molecule to be a harmonic oscillator. | [5] 2 | 3 |
| Q.2(b) Show that the R-branch lines get crowded and P-branch lines get widely spaced as J increases. | [5] 2 | 2 |
| Q.3(a) What are the differences between Born-Oppenheimer approximation and Franck-Condon principle? With clear schematics, discuss the role of Franck-Condon principle in predicting intensity of spectral lines of vibrational-electronic spectra. | [5] 3 | 2 |
| Q.3(b) Show that the symmetry of pi and n orbitals in formaldehyde and relevant transitions associated with it. | [5] 3 | 3 |

C_{2v}	E	C_2	$\sigma_v(xz)$	$\sigma_v'(yz)$		
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

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| Q.4(a) Explain the differences among the UPS, XPS and AES techniques. What is Koopman's theorem? What are the assumptions involved in Koopman's theorem? | [5] 4 | 2 |
| Q.4(b) Explain the UPS spectrum of argon. | [5] 4 | 2 |
| Q.5(a) Discuss all possible magnetic interactions (including hyperfine interaction) present in H-atom in the presence of an external magnetic field. | [5] 5 | 2 |
| Q.5(b) Explain different relaxation processes involved in NMR spectroscopy. | [5] 5 | 2 |

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