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22PHP209N

PSG COLLEGE OF ARTS & SCIENCE
(AUTONOMOUS)

MSc DEGREE EXAMINATION MAY 2025
(Second Semester)

Branch - **PHYSICS**

GROUP THEORY AND MOLECULAR SPECTROSCOPY

Time: Three Hours Maximum: 75 Marks

SECTION-A (10 Marks)
Answer **ALL** questions
ALL questions carry **EQUAL** marks (10 × 1 = 10)

Module No.	Question No.	Question	K Level	CO
1	1	Which of the following species possesses both C_3 and C_2 axes? (a) NH_3 (b) $[H_3O]^+$ (c) SO_3 (d) PCl_3	K1	CO1
	2	The number of classes for a C_{2v} point group is (a) 4 (b) 3 (c) 5 (d) 1	K2	CO1
2	3	The direct product of any one dimensional irreducible representation gives (a) One dimensional irreducible representation (b) Totally symmetric irreducible representation (c) Linear combination of irreducible representation (d) Multidimensional irreducible representation	K1	CO2
	4	The letter g is attached to the Mullikan symbol based on (a) The character with respect to σ_h (b) The character with respect to inversion operation (c) The character with respect to identity operation (d) The character with respect to C_2 axis	K2	CO2
3	5	The molecule which is IR inactive but Raman active is: (a) HCl (b) SO_2 (c) N_2 (d) H_2O	K1	CO3
	6	The fingerprint region in the IR spectrum is (a) 666-4000 cm^{-1} (b) 666-1400 cm^{-1} (c) 1400-4000 cm^{-1} (d) 4000-400 cm^{-1}	K2	CO3
4	7	The source of UV radiation used in UV-Visible spectrophotometer is (a) Xenon vapour lamp (b) Hydrogen vapour lamp (c) Halogen vapour lamp (d) Sodium vapour lamp	K1	CO4
	8	In the UV spectrum of cyclohexanone, the absorption at λ_{max} = 215 nm is due to the transition (a) $\sigma \rightarrow \sigma^*$ (b) $\sigma \rightarrow n$ (c) $\pi \rightarrow n$ (d) $\pi \rightarrow \pi^*$	K2	CO4
5	9	Which is used as a standard reference in ^{1}H-NMR spectroscopy? (a) DPPH (b) KBr (c) $CDCl_3$ (d) TMS	K1	CO5
	10	The signal(s) for a compound like X-CH_2-CH_2-Y will be: (a) One triplet (b) One singlet (c) Two triplets (d) Two singlets	K2	CO5

SECTION - B (35 Marks)
Answer **ALL** questions
ALL questions carry **EQUAL** Marks (5 × 7 = 35)

Module No.	Question No.	Question	K Level	CO
1	11.a.	Derive the group multiplication table of the symmetry operations of ammonia molecule.	K4	CO1
		(OR)		
	11.b.	Prove that diagrammatically H_2O molecule is abelian whereas NH_3 molecule is non-abelian.		

Cont...

2	12.a.	Assess the properties of irreducible representations using great orthogonality theorem.	K5	CO2
		(OR)		
	12.b.	Determine the symmetries of normal modes of vibrations of $POCl_3$ molecule.		
3	13.a.	(i) Distinguish between Rayleigh scattering, Stokes lines and anti-Stokes lines. (3) (ii) How would you distinguish the following pairs of compounds with the help of IR spectrum? (4) 1. CH_3CH_2OH and CH_3-O-CH_3 2. CH_3CH_2CHO and CH_3-CO-CH_3	K4	CO3
		(OR)		
	13.b.	(i) The reduced mass of a HCl is 1.626×10^{-27} kg and its vibrational frequency is $2890cm^{-1}$. Calculate the force constant. (3) (ii) An organic compound with molecular mass C_8H_{18} shows the following characteristic absorption bands: (ii) $2925cm^{-1}$ (st) (ii) 1465 cm^{-1} (iii) 1380 cm^{-1} (iv)$720cm^{-1}$. Determine the structure of the compound. (4)		
4	14.a.	Predict the various electronic transitions possible in the following compounds: (7x1=7) (i) CH_4 (ii) CH_3Cl (iii) HCHO (iv) Cl_2 (v) CH_3OH (iv) $CH_2=CH_2$ (vii) CH_3-CO-CH_3	K6	CO4
		(OR)		
	14.b.	(i) Predict the λ_{max} values of 2,4-Hexadiene. (3) (ii) Define the term 'chromophore'. How will you detect the presence of carbonyl group in aldehydes and ketones using UV-Visible spectroscopy? (4)		
5	15.a.	(i) ^{13}C is NMR active while ^{12}C is not. Justify this statement. (3) (ii) Compare first order and non- first order spectra in NMR. (4)	K5	CO5
		(OR)		
	15.b.	(i) Coupling between bonded ^{13}C's not a factor in ^{13}C-NMR spectroscopy. Validate this statement.(3) (i) Assess the effect of quadrupole nuclei on relaxation mechanism. (4)		

SECTION -C (30 Marks)

Answer **ANY THREE** questions

ALL questions carry **EQUAL** Marks (3 × 10 = 30)

Module No.	Question No.	Question	K Level	CO
1	16	Derive the matrix representation for rotation and reflection operations.	K4	CO1
2	17	Construct a character table for C_{2v} point group and also find the symmetries of normal modes of vibrations of water molecule.	K6	CO2
3	18	Deduct the instrumentation of Raman spectroscopy.	K5	CO3
4	19	(i) Evaluate the effect of solvent polarity on K and R-bands. (5) (ii) State Beer-Lambert's law. 2.5×10^{-5} M solution of a substance in a 1 cm length cell at λ_{max} 245 nm has absorbance 1.17, Calculate ε_{max} for this transition. (5)	K5	CO4
5	20	(i) Aromatic protons are more deshielded than ethylenic protons, although both the types of protons are attached to sp^2 hybridized carbon atom. Analyze this observation. (5) (ii) Examine the scalar spin-spin coupling mechanism of acidified ethanol. (5)	K4	CO5

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