B.SC. MSC INTEGRATED PROGRAMME
JAMIA HAMDARD
Semester VI Examination 2024
Paper code: Code-BCH-CC12TH
Title: BASICS OF QUANTUM CHEMISTRY AND SPECTROSCOPY
(Write your Roll No. at the top immediately on receipt of this question paper)

Time: **2.5 Hours** Maximum Marks: **75**

*Note: **Attempt all the questions marks of each question given in parenthesis. All parts of a question must be attempted in continuation. Start answer of a fresh question on a new page. Cite examples and draw labelled diagrams wherever necessary. Attempt all questions.** Use of Scientific Calculator is permitted.*

Q. No		BTL	CLO	PLO
Q1.	Attempt ***Any Ten*** of the following: Very Short Type Questions:	**(10 x 2 = 20 Marks)**		
	1. What are the selection rules in rotation spectroscopy?	1/2	1/2	1/2
	2. What is anharmonicity in vibrational spectroscopy?	1/2	1/2	1/2
	3. What are the P, Q, and R branches in vibration-rotation spectroscopy?	1/2	1/2	1/2
	4. What is the Franck-Condon principle in electronic spectroscopy?	1/2	1/2	1/2
	5. How are singlet and triplet states differentiated in electronic spectroscopy?	1/2	1/2	1/2
	6. What is chemical shift in NMR spectroscopy?	1/2	1/2	1/2
	7. What are the scales used in NMR spectroscopy to represent chemical shifts?	1/2	1/2	1/2
	8. Explain hyperfine structure in ESR spectroscopy.	1/2	1/2	1/2
	9. How is ESR spectroscopy applied to study simple radicals?	1/2	1/2	1/2
	10. Predict the proton- NMR spectrum of ethanol and HD along with deuteron-NMR spectrum of HD?	1/2	1/2	1/2
	11. Show that the commutator [x, $\frac{\partial}{\partial x}$]= -1.	1/2	1/2	1/2
	12. If $\hat{A}$ and $\hat{B}$] cap are two operators such that [$\hat{A}$, $\hat{B}$] = 1, show that [$\hat{A}$, $\hat{B}2$] = 2 $\hat{B}$.	1/2	1/2	1/2
	13. Show that $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$	1/2	1/2	1/2
	14. Explain Heisenberg uncertainty principle.	1/2	1/2	1/2
	15. Show that $[\hat{A}2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$	1/2	1/2	1/2
Q2.	Attempt **any two** of the following: Long answer type Questions:	**(2x10=20 Marks)**		
	1. How does the Morse potential model for anharmonic oscillators contribute to our understanding of molecular vibrations in spectroscopy?	5/6	5/6	5/6/7
	2. Find the expressions for the following operators: A. $(\frac{\partial}{\partial x} + x)^2$ B. $(\frac{\partial}{\partial x} - x)^2$ C. $(\frac{\partial}{\partial x} + x)((\frac{\partial}{\partial x} - x)$ D. $(\frac{\partial}{\partial x} - x)((\frac{\partial}{\partial x} + x)$	5/6	5/6	5/6/7
	3. Compare the bond energy, bond length, bond strength & magnetic character of O_2, O_2^+, O_2^-, and O_2^2 with the help of MOT.	5/6	5/6	5/6/7
	4. How many kinds of proton are there in $(CH_3)_2CHCH_2CH_3$ and $C_6H_5CH_3$, $C_6H_5NO_2$, $CH_2=CH_2$, $CH_3CH=CH_2$?	5/6	5/6	5/6/7

Q3.	Attempt the following: short answer type Questions:	(7x5=35 Marks)		
	1. The pure rotational (MW) spectra of spectra of gaseous HCl consist of a series of equally spaced lines separated by 20.80 cm^{-1}. Calculate the internuclear distance of the molecule. (Given the atomic masses ^{1}H= 1.673x10^{-27} Kg; ^{35}Cl= 58.06x10^{-27} Kg). **OR** Discuss the various postulates of quantum mechanics?	5/6	5/6	5/6/7
	2. Calculate the nuclear spin angular momentum and the magnetic moment for a proton, given that I =1/2, g_N for proton is 5.585 and μ_N= 5.05x10-27 JT^{-1}. Calculate the magnetic field strength required to observe the NMR frequency for fluorine (^{19}F) at 60 MHz. Given g_N for ^{19}F = 5.257 and μ_N = 5.05x10-27 J T^{-1}. **R** Show that the commutator $[\widehat{Xn}]$, $\widehat{px}]=\frac{ih}{2}$ n x^{n-1} where n is a positive integer.	4/5/6	4/5/6	4/5/6
	3. How does the "Particle in a One-Dimensional Box" model illustrate the concept of quantized energy levels and their relationship to particle confinement within a limited space? **OR** In an ESR spectrometer, the ESR frequency of the free electron is 9.5 GHz. Calculate the magnetic field at which the spectrometer is operating, g_e = 2 and u_B = 9.273 x 10^{-24} J T^{-1}? Differentiate the proton- NMR spectrum of NH_3 from that of NH_4^+ ion?	5/6	4/5/6	4-7
	4. Which of the following molecule will show a spectrum and why? Type of spectrum | Molecules Pure rotational (MW) | H_2, HCl, CO, $CHCl_3$, H_2O, NH_3, and NH_4Cl Vibrational (IR) | H_2, HCl, CO, $CHCl_3$, H_2O, NH_3, NH_4Cl, CH_3-CH_3, C_6H_6, CCl_4, and CO_2 Rotational Raman | H_2, HCl, CO, CH_4, $CHCl_3$, H_2O, NH_3, CH_3-CH_3, and SF_6 Vibrational Raman | H_2, HCl, CO, CH_4, $CHCl_3$, H_2O, NH_3, CH_3-CH_3, and SF_6 **OR** How does the '1-D Simple Harmonic Oscillator' model, as applied in quantum chemistry, help explain the vibrational motion and energy quantization of molecules, and what are its implications for understanding molecular properties?	3-5	3-6	3-5
	5. What are the key differences between Molecular Orbital Theory and Valence Band Theory regarding their explanations of electronic structure and bonding in materials? **OR** The fundamental vibration of HCl is 2890 cm^{-1}. Calculate the force constant of this molecule. (Given the atomic masses ^{1}H= 1.673x10^{-27} Kg; ^{35}Cl= 58.06x10^{-27} Kg).	3-5	3-5	3-5
	6. Draw the molecular orbital diagram of Hetronuclear diatomic molecule (CO, NO, HF), HCl. Write the electronic configurations of H_2, H_2^+ and the hypothetical species H_2^- in terms of molecular orbital theory. Why does He+ exist whereas He_2 does not? **OR** Explain the Bathochromic, Hypsochromic, Hypochromic and Hyperchromic Shift?	3-5	3-5	3-5
	7. What are Different types of spectra given by a molecule and what is Stark effect in MW spectra? **OR** Assuming that the ionic character in H-Br bond is 11%, calculate the fraction of the contribution of ionic character to the valence bond wave function.	3-5	3-5	3-5