B.Sc. (H) Chemistry, Semester- V (2023- 24)
Internal Assessment Test
Paper- Quantum Chemistry and Spectroscopy

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*Attempt any **five** questions.* ***MM = 2 × 5 = 10***

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1. Which of the following are eigen function of $\frac{d^2}{dx^2}$ operator:
   Sin 3x, 6 cos 4x, 5 x^2, 3 e^{-5x}.
2. Evaluate the commutator: $[\widehat{L_x}, \widehat{L_y}]$.
3. The fundamental vibrational frequency of CO is 2170.2 cm^{-1}. Calculate the force constant of the molecule.
4. There exists a set of orthogonal functions which are simultaneously eigen function of both the operators $\hat{A}$ and $\hat{B}$. Prove that $\hat{A}$ and $\hat{B}$ must commute for this statement to be true.
5. Why n = 0 is not permitted for wave function for particle in a box?
6. Show that $\psi = \sqrt{\frac{2}{a}} \sin \frac{n \pi x}{a}$ is not an eigen function of linear momentum operator.
7. For $^{1}H^{79}Br$, the rotational constant B, is found to be 8.45 cm^{-1}. Draw the rotational energy level diagram for J = 1, 2, 3, 4.