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

CLASS: IMSC | **SEMESTER : V**
BRANCH: CHEMISTRY | **SESSION : MO/2022**

SUBJECT: CH301 PHYSICAL CHEMISTRY-V: QUANTUM CHEMISTRY & SPECTROSCOPY

TIME: 3:00 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.

Q.1(a) Why does IR spectrum appear as band whereas rotational spectrum appears as line? [2]
Q.1(b) Show that, the spacing between two successive lines in rotational spectrum of a diatomic molecule is 2B where B is a rotational constant. [3]
Q.1(c) The rotational constant for $H^{35}Cl$ is observed to be 10.5909 cm^{-1}. What is the value of B for $H^{37}Cl$? [5]

Q.2(a) How does IR spectrum help in the detection of functional groups and bond distance? [2]
Q.2(b) Discuss the theory to explain Rayleigh, stokes and anti-stokes lines in the Raman spectrum. [3]
Q.2(c) Explain why H_2 is Raman active whereas microwave and IR inactive? [5]
What are the advantages of Raman spectroscopy over IR spectroscopy?

Q.3(a) Why electronic spectrum is a band spectrum? [2]
Q.3(b) Explain the Frank Condon principle. [3]
Q.3(c) How many lines can be seen for the following molecules in ^1H NMR spectroscopy? Mention the nature of splitting also. [5]
$CH_3CH_2CH(OH)CH_2CH_3$ $(CH_3)_2CHCOCH_3$ $(CH_3)_2CHCH_2CHO$

Q.4(a) For a particle in a one dimensional box of Length L, find the probability, in the states n=1, 2 and 3, that the particle is in the region $0 \le x \le L/4$. [3]
Q.4(b) Which of the following functions are acceptable as wave function: i) $\varphi = x^2$ ii) $\varphi = tanx$ iii) $\varphi = exp^{-x}$ iv) $\varphi = sinx$ [2]
Q.4(c) Evaluate the following i) $[L_x, L_y]$=? and ii) $[L^2, L_y]$=? [5]

Q.5(a) Show how the Hamiltonian for the H atom could be written in terms of the internal motions by considering separation of the translational and internal motions. [3]
Q.5(b) Show that the following function is a solution of the Schrodinger equation for a simple harmonic oscillator i) $\varphi = exp^{-ax^2}$. Find the values of ii) a and iii) energy (E) in terms of force constant (k), mass (m) and the universal constant. [3]
Q.5(c) Considering the nuclei to be fixed in space, write down the Hamiltonian for H_2^+. Derive an expression for energy levels (ground and first excited state) by constructing a suitable trial function for this system by following variational principle. [4]

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