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

**CLASS: M.Sc. / IMSc** **SEMESTER : II /VIII**
**BRANCH: Chemistry** **SESSION : SP/22**

**SUBJECT: CH409 Physical Chemistry-VII: Quantum Chemistry & Group Theory**
**TIME: 02 hrs** **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) For a particle in a 1D box of length 1 Å, what will be the wavelength of the wave associated with n = 2 state? For the two states (n = 1 & n = 2) particle in a 1D box, find the values of eigenfunctions at several values of x between – L/2 and + L/2. [2+3]

Q.1(b) Explain zero-point energy for particle in 1-D box. Show the non-degenerate and degenerate states for three dimensional cubical box with energy levels diagram. [2+3]

Q.2(a) Describe and prove the Variational Theorem. [5]

Q.2(b) Utilizing time-independent perturbation theory, derive an expression for the first order correction to the wave function. [5]

Q.3(a) (i)Write down the Slater determinant for a Li atom. (ii) What is meant by a Fermi hole? [2+3]

Q.3(b) (i) Explain in detail about the Fock operator. (ii) What is a Permutation operator? [3+2]

Q.4(a) Write down the Born Oppenheimer approximation. Explain the LCAO approximation. [3+2]

Q.4(b) Construct the character table for $C_{2v}$ point group with proper explanation. [5]

Q.5(a) Write down the postulates of Great Orthogonality Theorem? A group has the following irreducible representations: $A_1$, $A_2$, $B_1$, $B_2$, $E_1$, $E_2$. (i) What is the order of the group? (ii) How many classes are in the group? [3+1+1]

Q.5(b) Discuss the principle of reduction of reducible representation into irreducible representation taking water as an example. [5]

**:::::29/04/2022 E:::::**