

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

CLASS: MSC/IMSC/PRE-PHD
BRANCH: CHEMISTRY

SEMESTER : II/VIII/NA
SESSION : SP/2023

SUBJECT: CH409 QUANTUM CHEMISTRY & GROUP THEORY

TIME: 3 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.
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		CO	BL
Q.1(a)	Explain the variational theorem.	[3]	5 2
Q.1(b)	Considering time-dependent perturbation theory, derive an expression for the transition probabilities between states. Using your results obtained herein, explain how time-dependent perturbation theory could be used to understand interaction between light and matter and thereby emission and absorption spectroscopy.	[3+4]	5 3
Q.2(a)	Consider a particle moving in a 1 Dimensional box. This particle is subjected to a uniform electric field of strength Ω as a result of which its potential energy increases linearly with x . Find the lowest energy eigenvalue for this particle.	[3]	5 2
Q.2(b)	Discuss the Born-Oppenheimer approximation. Derive an expression for the Nuclear Schrodinger equation by starting from the total molecular Hamiltonian and by considering both nuclear and electronic parts of the total wave function for a given system.	[2+5]	5 3
Q.3(a)	Explain what is meant by a Fock operator. Write down the Slater determinant for a Li atom.	[2+2]	5 2
Q.3(b)	Consider the following spin (part of the) wave function: $N[\alpha(1)\beta(2) - \alpha(2)\beta(1)]$. Show whether this state could be considered as a pure spin state or not.	[6]	5 3
Q.4(a)	What is the point group of tetrachloropalladate $[\text{PdCl}_4]^{2-}$ and show the symmetry elements. For water molecule, $\Gamma_1 = 3A_1 + A_2 + 3B_1 + 2B_2$, find out the different modes of vibration which are IR active, Raman active & both IR and Raman active.	[2+3]	5 3
Q.4(b)	Discuss the principle of reduction of reducible representation into irreducible representation taking water as an example.	[5]	5 2
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+2]	5 3
Q.5(b)	Construct the character table for NH_3 molecule with proper explanation.	[5]	5 3

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