

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

CLASS: MSc
BRANCH: CHEMISTRY

SEMESTER : II
SESSION : SP/2025

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)	Calculate the energy of a particle in a 1D-box of length L.	[5]	1 1
Q.1(b)	Obtain the wave function of a particle in a 1D-box of length L.	[5]	2 2
Q.2(a)	Derive the form for the first order correction to energy using Rayleigh-Schrodinger perturbation theory.	[5]	1 1
Q.2(b)	Describe the Linear variational method.	[5]	2 2
Q.3(a)	Derive the ground state electronic term symbol for C.	[5]	2 2
Q.3(b)	Derive the ground state electronic term symbol for Pb.	[5]	3 3
Q.4(a)	State and explain Born-Oppenheimer approximation.	[5]	1 1
Q.4(b)	Discuss ion-covalent resonance.	[5]	1 2
Q.5(a)	Consider three symmetry elements: E, X, Y. Construct the corresponding group multiplication table for these. Write down the matrix representation of improper rotation.	[3+2]	2 2
Q.5(b)	Assign point group to the following molecules: NH ₃ , H ₂ O.	[5]	2 3

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