



THE AMERICAN COLLEGE

an Autonomus Institution affiliated to the Madurai Kamaraj University

Re- accredited (2nd Cycle) by NAAC with Grade "A"

CGPA-3.46 on a 4-point scale

BACKLOG ARREAR EXAMINATION- MARCH 2021

DEPARTMENT OF CHEMISTRY

PGC4405

PHYSICAL CHEMISTRY-I

Time: 3 Hours

Max Marks: 75

Answer ANY FIVE Questions

(5 X 15 = 75)

1. a) Explain with suitable example the commutative operator. (5) b) Set up the Schrodinger wave equation and solve it for the rigid rotor problem.(10)
2. Discuss variation method for obtaining approximate value of ground state energy of He atom. (12). Compare the results with that obtained from perturbation method. (3)
3. a) Describe Hartree Fock self-consistent field method. (10) b) Describe the quantum mechanical approach to Pauli exclusion principle. (5)
4. a) What is meant by similarity transformation? (3). How is this property used to obtain the class present in a group? (7) b) State and explain great orthogonality theorem. (5)
5. Find out the symmetries of normal modes of ammonia and predict using group theory the vibrations which are IR active and Raman active. (15)
6. Apply MO theory and obtain energy and eigen function for hydrogen molecule. (15)
7. a) Construct the C_{2h} character table. (8) b) What are term symbols? Arrive at the term symbol for any two systems. (7)

Signature of the Internal Examiner

Scheme of valuation

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1. a) commutative operator relation- 3. Explanation-2 (5) b) Set up the Schrodinger wave equation for the rigid rotor problem (2) and solve it for wavefunction (4), energy with diagram (4) (10)
2. Discuss variation method for obtaining approximate value of ground state energy of He atom. (12). Compare the results with that obtained from perturbation method. (3)
3. a) Hartree Fock self-consistent field method explanation -5, illustration -5. (10) b) Describe the quantum mechanical approach to Pauli exclusion principle. (5)
4. a) What is meant by similarity transformation? (3). How is this property used to obtain the class present in a group? (7) b) State and explain great orthogonality theorem. (5)
5. Find out the symmetries (7) of normal modes of ammonia and predict using group theory the vibrations which are IR active (4) and Raman active. (4). (15)
6. Apply MO theory and obtain energy and eigen function for hydrogen molecule. (15)
7. a) Construct the C_{2h} character table. (8) b) What are term symbols? (3) Arrive at the term symbol for any two systems. (2+2) (7)

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