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

PGC4425　　　　　**PHYSICAL CHEMISTRY-I**　　　　　**Time: 3 Hours**

Max Marks: 75

Answer **ANY FIVE** Questions　　　　　**(5 X 15 = 75)**

1. Set up Schrodinger wave equation for hydrogen atom and separate it into the radial and angular parts, solve the radial part of the equation to obtain energy and quantum numbers. (15)

2. Discuss perturbation method for obtaining approximate value of ground state energy of He atom. (12). Compare the results with that obtained from variation 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. Deduce symmetrically using water molecule as example, the active vibrational modes in IR and Raman spectra using group theory (15)

6. a) Using group theory obtain SALC and Pi energy for benzene system. (8) b) Construct character table for C_5 point group. (7)

7. a) Calculate the Huckel pi-electron energies of cyclobutadiene. (8) b) What are term symbols? Arrive at the term symbol for any two systems. (7)

Signature of the Internal Examiner

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PGC4425 **PHYSICAL CHEMISTRY-I** **Time: 3 Hours**
Max Marks: 75

Answer **ANY FIVE** Questions **(5 X 15 = 75)**

1. Set up Schrodinger wave equation for hydrogen atom (3) and separate it into the radial and angular parts, (2) solve the radial part of the equation to obtain energy (3x2=6) and quantum numbers. (4) = (15)

2. Discuss perturbation method for obtaining approximate value of ground state energy of He atom. (12). Compare the results with that obtained from variation 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. Deduce symmetrically (5) using water molecule as example, the active vibrational modes in IR (5) and Raman spectra (5) using group theory (15)

6. a) Using group theory obtain SALC and Pi energy for benzene system. (8) b) Construct character table for C_5 point group. (7)

7. a) Calculate the Huckel pi-electron energies of cyclobutadiene. (8) b) What are term symbols? (2) Arrive at the term symbol for any two systems (2.5x2). (7)

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