

PSG COLLEGE OF ARTS & SCIENCE  
(AUTONOMOUS)

MSc DEGREE EXAMINATION DECEMBER 2018  
(Second Semester)

Branch-CHEMISTRY

PHYSICAL CHEMISTRY - II

Time : Three Hours

Maximum : 75 Marks

Answer ALL questions  
ALL questions carry EQUAL marks (5 x 15 = 75)

- 1 a Show that  $x$  and  $\frac{d}{dx}$  operators do not commute each other. Give its significance. (5)
- b Derive the operators for linear momentum and energy. (10)
- OR
- c State and explain Hermitian operators. (5)
- d Describe the essential postulates of quantum mechanics. (10)
- 2 a Derive the Schrodinger wave equation for particle in 1D box and obtain the energies and normalized wave functions. (10)
- b Sketch and explain the radial wave functions. (5)
- OR
- c Apply quantum mechanics to He atom problem and solve it to get eigen values, functions and quantum numbers. (15)
- 3 a Write the Slater determinants for He atom. (5)
- b State and explain first order perturbation theory. (5)
- c Give the application of perturbation theory to He atom. (5)
- OR
- d State and explain variation method. (5)
- e Describe the salient features of Hückel MO theory and its application to benzene. (10)
- 4 a Obtain the matrix representations of symmetry operations. (7)
- b What are space groups? Give examples. (4)
- c Sketch and explain the symmetry elements and operations in water molecule. (4)
- OR
- d State and explain great orthogonality theorem. (5)
- e Apply the great orthogonality theorem and construct the character table for  $C_{3v}$  point group. (10)
- 5 a Explain the symmetry based selection rules for IR and Raman spectra. (8)
- b Determine the vibrational modes in  $H_2O$  using group theory. (7)
- OR
- c Discuss the construction of hybrid orbitals of  $BF_3$  and  $NH_3$  molecules