

PG/Chem/3rd Sem/21(CBCS)

2021

CHEMISTRY
Paper : CHEM-301
(Physical Chemistry)
(CBCS)

Full Marks : 40

Time : Two Hours

The figures in the margin indicate full marks.

Question No.1 is compulsory and answer any three from the rest.

1. Answer any *five* of the following : 2×5=10

- (a) Evaluate $[\hat{x}, \hat{H}]$
- (b) Find $Y_l^m(\theta, \Phi)$ for $l = 0$ and $l = 1$.
- (c) State and explain the variation principle.
- (d) What are Einstein coefficient A and B? State their units.
- (e) For $S = \frac{1}{2}$, find $\langle \alpha | S_z | \alpha \rangle$ and $\langle \alpha | S_x | \beta \rangle$.
- (f) State and explain *Koopman's* theorem.
- (g) What is radial distribution function?
- (h) What is a *ladder* operator? Give an example.

2. (a) Write the operator L_z in Cartesian as well as in polar coordinates. State its unit. Find the eigenfunction of the operator. Comment on the value of the quantum number associated with the eigenfunction. 6

- (b) Find the energy expression of a rigid rotor. 4
3. (a) Write the Schrodinger equation for the electronic part of a hydrogen atom and separate it into radial and angular parts. 4
- (b) Show that the hydrogen like atomic wave function ψ_{210} is normalized and that is orthogonal to ψ_{200} . 3
- (c) The 1s orbital of a H atom is given by $\phi(r) = A \exp(-r/a)$ where A and a are constant. Find the most probable value of r . 3
4. (a) Apply the principle of linear variation to find the pi-MO of ethylene. 4
- (b) Using time dependent perturbation theory derive the *Fermi Golden Rule*. 6
5. (a) Comment on the symmetry property of a many electron wave function with respect to interchange of electrons. State and explain *Pauli Exclusion Principle*. 4
- (b) Write the spin operators S_x , S_y and S_z in matrix representation. Show by matrix multiplication that $[S_x, S_y] = i\hbar S_z$. 4
- (c) Explain what is meant by a *Slater* determinant? Give an example. 2
6. (a) Explain what are *Coulomb and exchange* operators. 4
- (b) Explain the *Born Oppenheimer approximation*, State its use in finding the molecular energy levels. 4
- (c) Explain the term *correlation energy*. 2
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