

TDC (CBCS) Odd Semester Exam., 2021
held in March, 2022

CHEMISTRY

(5th Semester)

Course No. : CHMHCC-502T

(Physical Chemistry—V)

Full Marks : 50

Pass Marks : 20

Time : 3 hours

*The figures in the margin indicate full marks
for the questions*

SECTION—A

Answer any *ten* from the following : 2×10=20

1. Write two postulates of quantum mechanics.
2. Show that Hermitian operators have real eigenvalues.
3. If \hat{A} and \hat{B} are two operators such that $[\hat{A}, \hat{B}] = 1$, then find the value of $[\hat{A}, \hat{B}^2]$.

4. Define exchange and Coulomb integrals.
5. Calculate the most probable distance of the electron from the nucleus in the ground state of H-atom.
6. Calculate the bond order of CN^- . Which one, CO^+ or O_2 will be stabilized by removal of an electron? 1+1=2
7. Discuss the effect of UV and IR radiations on the molecule.
8. How does the change in bond length of diatomic molecule affect the rotational spectra of the molecule?
9. Explain why homonuclear diatomic molecule does not show vibrational spectra.
10. Explain why Stokes lines are more intense than anti-Stokes lines.
11. What is fluorescence? Why does fluorescence occur much faster than phosphorescence?

12. What do you mean by spin-spin coupling in high resolution spectra of NMR spectroscopy?
13. State the two laws of photochemistry.
14. What is photosensitized reaction? Give one example each of natural and artificial photosensitized reactions. 1+1=2
15. Define the term 'chemiluminescence'. Give an example.

SECTION—B

Answer any *five* from the following : 6×5=30

16. (a) Solve the Schrödinger wave equation for a particle of mass m moving in a three-dimensional (3-D) cubical box with edge of length a . 3
- (b) What is degeneracy? Calculate the degree of degeneracy for the energy level $\frac{14h^2}{8ma^2}$. 1+2=3

17. (a) Write and solve the Schrödinger's wave equation for a one-dimensional (1-D) simple harmonic oscillator (SHO). 5
- (b) What is zero-point energy? 1
18. Set up Schrödinger's wave equation in spherical polar coordinates for H-atom and hence separate it into radial and angular parts. 6
19. Write the Hamiltonian operator for H_2^+ in terms of MOT and hence solve the Schrödinger's wave equation for H_2^+ to determine the secular equations. 6
20. (a) Explain the intensity curve of pure rotational molecule. 3
- (b) Obtain an expression of energy for vibrating diatomic molecule. 3
21. (a) Explain mutual exclusion principle with an example. 3
- (b) Explain the origin of P, Q, R branches of line in vibrational-rotational spectra. 3

22. (a) State and explain Franck-Condon principle of electronic transition. 3
- (b) Explain the PMR spectra of $\text{CH}_3 - \text{CH}_2 - \text{OH}$. 3
23. (a) Discuss the effect of solvent polarity and conjugation on the absorption maxima of a compound. 3
- (b) Explain the principle of NMR spectroscopy. 3
24. (a) Define quantum yield. Give two reactions each for high and low quantum yields of photochemical reactions. 1+2=3
- (b) Explain the physical significance of absorption coefficient. 3
25. (a) Explain various photophysical processes in detail giving Jablonski diagram. 5
- (b) What is quenching? 1

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