TDC (CBCS) Odd Semester Exam., 2023

CHEMISTRY

(Honours)

(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 *ten* questions, selecting any *two* from each Unit : 2×10=20

UNIT—I

1. Prove that the linear combination of two well-behaved functions is also a well-behaved function.

2. Write the expression for frequency of vibration in classical mechanics and draw the potential energy diagram of the expression $V = \frac{1}{2}kx^2$.

3. What do you mean by rigid rotor? Write the expression for energy of a rigid rotator.

UNIT—II

4. Set up the Schrödinger equation for the many-electron atoms and outline the factors which prevent a direct solution of this equation.

5. Write the Hamiltonian for hydrogen molecule using MOT, giving the meaning of the terms involved.

6. State and explain variation theorem.

UNIT—III

7. Which of the following molecules will show a pure rotational spectrum?

H_2, HCl, H_2O, CH_4, CH_3Cl, NH_3, CO

8. Write Born-Oppenheimer approximation.

9. The pure rotational spectra of HI consist of a series of lines separated by $13{\cdot}10\ cm^{-1}$. What is the bond length of the molecule?

UNIT—IV

10. What are the differences between Rayleigh scattering and Raman scattering? What are Stokes lines and anti-Stokes lines?

11. What is NMR spectroscopy? How does NMR-spectroscopy differ from UV- and IR-spectroscopy?

12. State Franck-Condon principle. Give its wave mechanical formulation.

UNIT—V

13. State and explain Lambert-Beer law.

14. What is an einstein? Determine the value of one einstein for a light of wavelength 200 nm in *(a)* SI unit and *(b)* calories.

15. Write a brief note on fluorescence.

SECTION—B

Answer *five* questions, selecting *one* from each Unit : 6×5=30

UNIT—I

16. *(a)* Calculate the zero-point energy of an electron confined to one-dimensional box of length 1·5 nm. 2

(b) Solve the Schrödinger wave equation for a particle in a 3-D box of volume a^3 and find the expression for the energy. 4

17. Write the Schrödinger wave equation for 1-D simple harmonic oscillator and solve it to the complete solution. What is its zero-point energy? Is it in accordance with Heisenberg uncertainty principle? 4+1+1=6

UNIT—II

18. Apply LCAO-MO theory to H_2^+ ion to derive the secular determinant. Solve it, find the energy levels and the corresponding normalized wave function. 4+1+1=6

19. Write down the Schrödinger equation for H-atom in spherical polar coordinate and separate it into r, θ and ϕ dependent equations. 6

UNIT—III

20. (a) Define rotational constant. Show that rotational energy difference between the ground-state and the first level is equal to twice the rotational constant expressed in cm^{-1}. 3

(b) The vibrational spectrum of HI has lines $12{\cdot}8\ cm^{-1}$ apart. Calculate moment of inertia and bond length of HI. 3

21. (a) Explain the formations of P, Q and R branches of a vibrating rotator. 3

(b) Draw a tabular scheme to show the different regions of electromagnetic radiation. 3

UNIT—IV

22. (a) What is Raman effect? Discuss the mechanism of Raman effect. 2+2=4

(b) Define singlet and triplet states of electron. 2

23. (a) Explain how shielding and deshielding affect the NMR spectra. 3

(b) Explain the NMR spectra of ethanol under low and high resolutions. 3

UNIT—V

24. (a) Draw a neat Jablonski diagram, explaining the various photochemical processes. 3

(b) A system absorbs 2×10^{16} quanta of light per second. At the end of 10 minutes it is observed that only 0·001 mol of the irradiated light has reacted. What is the quantum efficiency of the process? 3

25. (a) State and explain Einstein-Stark law of photochemical equivalence with suitable example. 3

(b) Define quantum yield. Give two reactions each for high and low quantum yields of photochemical reactions. 1+2=3

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