Reg. No..... Name.....

B.SC. DEGREE END SEMESTER EXAMINATION OCTOBER 2016

SEMESTER – 5: CHEMSITRY (CORE COURSE)

COURSE: U5CRCHE8 – QUANTUM MECHANICS AND SPECTROSCOPY

Time: Three Hours Max.Marks: 60

SECTION A

Answer ***all*** the questions. Each question carries ***1*** **mark**

1. The minimum frequency required for a light to cause ejection of photoelectron from the surface of a metal is called.....
2. Write de Broglie's equation.
3. Number of fundamental vibrational frequencies in CO_2 molecule is _____.
4. Define zero-point Energy.
5. What are the possible electronic transitions in acetone?
6. What is quantum yield?

State whether the following statements are true or false. Rationalize your answer.

7. HCl gives IR spectrum.
8. C-H proton is more deshielded than O-H proton (1 x 8 = 8)

SECTION B

Answer ***any Six*** questions. Each question carries **2 marks**

9. What is chemical shift?
10. Describe with examples (a) bathochromic shift (b) hypsochromic shift
11. Explain Davisson and Germer experiment.
12. Prove that uncertainty principle can be disregarded in the case of a cricket ball weighing 100 g is to be located with in 0.1 A^o.
13. What is McLafferty rearrangement?
14. Why is TMS used as a standard reference in NMR?
15. Pure rotational spectrum of a gaseous molecule consists of equally spaced lines separated by 41.60 cm^{-1}. Calculate the moment of inertia of the molecule.
16. What is Raman scattering? (2 x 6 = 12)

SECTION C

Answer **any *Four*** questions. Each question carries ***5*** **marks**

17. Write the postulates of Quantum mechanics.
18. Describe quantum numbers with their significance.

19. Explain Frank Condon principle.

20. Draw and discuss the high resolution NMR spectra of anhydrous ethanol and aqueous ethanol

21. Write notes on the factors affecting the width and intensity of spectral lines.

22. The hydrogen halides have following fundamental vibrational frequencies: $H^{35}Cl$ (2988.9 cm^{-1}); $H^{81}Br$ (2649.7 cm^{-1}). Calculate the force constants for the hydrogen-halide bonds. (5 x 4 = 20)

SECTION D

Answer **any *Two*** questions. Each question carries **10 marks**

23. Describe the principle and functioning of mass spectroscopy. Explain the basic fragmentation pattern taking 2-methyl butane as example.

24. Derive the expression for energy of particle in one-dimensional box and apply this to butadiene system.

25. (a) Explain fluorescence, phosphorescence and non-radiative processes using Jablonsky diagram

(b) Explain photosensitized reactions with 2 examples

26. (a) Derive the equation for rotational energy of a rotating diatomic molecule

(b) Write short notes on i) fundamental frequency ii) overtones iii) hot bands (10 x 2 = 20)

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