FIRST SEMESTER M.Sc. DEGREE EXAMINATION, DECEMBER 2014

(CUCSS)

Chemistry

CH 1C 01—THEORETICAL CHEMISTRY – I

(2010 admissions)

Time : Three H   Maximum : **36** Weightage

Section A

Answer all questions.
Each question carries a weightage of 1.

1. Which o ;he following are well behaved functions ? Justify your answer.

   (a) ax^2 (x **varies from 0 to** 00).

   (b) $\sin^{-1} x$ (x varies from -1 to +1).

2. Find the commutator of x and $\dfrac{d}{dx}$.

3. Which of the following are **eigen** functions of $\dfrac{d}{dx}$. Justify your answer.

   (a) Sin x.   (b) Sin ^1x.

   (c) e^{ax}.   (d) e^-

4. Write recursion formula. Explain it significance.

5. Express $\hat{L}_z$ in Cartesian and spherical polar co-ordinates.

6. Define spherical harmonics. Write one example.

7. What do you mean by space quantization ? Explain.

8. State and explain postulate of spin by Goudsmith.

9. State and explain independent particle model !

10. State and explain variation theorem.

11. Define 'spin orbital'. Write one example.

                                           (14 x 1 = 14 weightage)

Turn over

12. Explain the term 'STO'.

13. Write trial wave function to understand binding in H_2 by VB method.

14. What is Coulomb operator ? Explain its significance.

(14 x 1 = 14 weightage)

Section B

Answer any **seven** *questions.*
Each question carries a weightage of 2.

15. Write Hamiltonian operator. Show that it is a Hermitian operator.

16. A particle is confined to one dimensional box of length a. Show that $\Delta x \times \Delta P x \quad \dfrac{L}{\quad}$,

$$w\chi = \frac{2}{a} \sin\left(\frac{\pi}{a}\right) x$$

17. For a rigid rotator L2 and Hamiltonian have the same set of eigen functions. Justify the statement.

18. Find the ground state energy of a particle confined to one dimensional box by variation method. Use the trial function $\phi = x(x - a)$. a is the length of the box.

19. Find the ground state energy of He by first order perturbation method.

20. Briefly discuss Roothan's concept of basis functions.

21. Consider bonding in CO and draw correlation diagram. Discuss.

22. An electron is confined to a cubical box of size 10 nm. Calculate the wavelength of the radiation required for a transition from (111) level to (211) level. Electron mass is 9.1 x 10^{-31} kg.

23. Find the charge density on Carbon atoms in butadiene. The π molecular orbitals are :

$$= 0.3717 \quad + 0.6017\, p_2 + 0.60\ 17\ p_3 + 0.3717\ \mathbf{p4}$$
$$4)2 = \mathbf{0.6017} \quad + 0.3717\, p_2 - 0.3717\ p_3 + 0.6017\ p_4$$
$$4)3 = 0.6017\ P_1 - 0.3717\ P_2 - 0.3717\ p_3 + 0.6017\ \digamma_4$$
$$\phi_4 = 0.3717 \quad - 0.6017\, p_2 + 0.6017\ p_3 - 0.3717\ \mathbf{p4}$$

24. Write a brief account of quantum mechanical treatment of SP$^\wedge$ hybridization.

(7 x 2 = 14 weightage)

Section C

*Answer any•**two** questions.*
Each question carries a weightage of 4.

25. Apply Schrödinger wave equation for one dimensional simple harmonic oscillator. Find eigen functions and eigen values.

26. Discuss briefly self consistent field method to solve many electron atoms.

27. Find lowest energy π bonding molecular orbital in benzene using HMO method.

28. Discuss briefly LAAO method of bonding on applied to hydrogen molecule ion.

(2 x 4 = 8 weightage)