STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86
(For candidates admitted during the academic year 2006–07 & 2007-08)

SUBJECT CODE: CH/PC/QG34

M.Sc. DEGREE EXAMINATION, NOVEMBER 2008
BRANCH IV- CHEMISTRY
THIRD SEMESTER

REG.NO .....

COURSE : MAJOR CORE
PAPER : QUANTUM CHEMISTRY AND GROUP THEORY
TIME : 30 MINUTES **MAX.MARKS : 20**

SECTION – A **(20x1=20)**

Answer all the questions:

I Choose the correct answer :

1. Which one of the following is a linear operator?
   a) log b) sin c) $\frac{d}{dx}$ d) $\sqrt{\ }$

2. Choose the function that is not hermitian:
   a) $\frac{d}{dx}$ b) $\frac{h}{2\pi i}\frac{d}{dx}$ c) $ih\frac{d}{dx}$ d) $\frac{d^2}{dx^2}$

3. The term ^3P state can be assigned to the ground state of which atom?
   a) Na b) C c) Mg d) Al

4. The SI unit of the wave function of a free particle moving in three dimension is
   a) m^{-1} b) $m^{-1/2}$ c) $m^{-3/2}$ d) m

5. Which one among the following constants has the same unit as that of angular momentum?
   a) Molar gas constant (R) b) Boltzmann constant (k)
   c) Planck's constant (h) d) Stefan-Boltzmann constant (σ)

6. The operator for the x - component of kinetic energy (T_x) of a system is
   a) $-\frac{h^2}{8\pi^2 m}\frac{\partial}{\partial x}$ b) $-\frac{h^2}{8\pi^2 m}\frac{\partial^2}{\partial x^2}$ c) $-\frac{h}{8\pi i}\frac{\partial}{\partial x}$ d) $-\frac{h}{2\pi i}\frac{\partial}{\partial x}$

7. The symmetry operation S_6^2 is equivalent to
   a) S_3^1 b) E c) C_3^2 d) C_3^1

8. Which one of the following molecules belongs to D_{2d} point group?
   a) Naphthalene b) Ferrocene c) Allene d) Benzene

9. In C_{2v} point group the product $C_2.\sigma_{xz}$ is equal to
   a) E b) C_2 c) σ_{yz} d) σ_{xz}

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10. In which one of the following molecule IR active modes are Raman inactive and Raman active modes are IR inactive?
a) Boric acid b) Boron trifluoride c) trans – dichloroethene d) chloroform

II Fill in the blanks :

11. XeF_4 belongs to _____ point group.
12. The sum of the square of the characters of any irreducible representation is equal to _____ of the group.
13. The symmetries of fundamental modes in H_2O molecule are _____.
14. The ionisation potential of Li in au is 0.2. The value of IP in eV is _____.
15. The ground state electronic configuration of molybdenum $(Z = 42)$ is _____.

III Answer in a line or two:

16. Write the x-component angular momentum operator $\left(\hat{L}_x\right)$.
17. What is inversion operator?
18. What is rule of mutual exclusion?
19. State Aufbau principle.
20. Write the expression for the eigen value of a rigid rotor.

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TIME : 2½ HOURS **MAX.MARKS : 80**

SECTION – B **(5 x 8 = 40)**

Answer any five questions :

1. State and explain Heisenberg's uncertainty principle. Calculate the uncertainty in velocity of an electron $(m = 9.1\times10^{-31}\ kg)$ that can be located with an accuracy of $0.01\ nm$.

2. State the postulates of quantum mechanics.

3. Apply perturbation theory to helium atom and obtain its energy in the ground state.

4. Explain Russel-Saunders coupling. Illustrate with two examples, how it can be applied to get the term symbols.

5. Write the ground state wave function for helium atom in the determinantal form and explain Pauli exclusion principle.

6. Write the group multiplication table for C_{3v} point group. Is it an abellian group?

7. Construct the character table for C_{2v} point group.

8. The reducible representation for a square planar molecule AB_4 is given below.

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
Γred	15	1	-1	-3	-1	-3	-1	5	3	1

Break it into irreducible represetation and obtain the symmetries of modes of vibration in AB_4. Predict their IR and Raman activity. (use of character table for D_{4h} is allowed)

SECTION – C **(2 x 20 = 40)**

Answer any two questions:

9. a) Show that the wave function $\Psi_{(x,y,z)} = \sin ax\ \sin by\ \sin cz$ (where a, b, c are constants) is an eigen function for Laplacian operator. Find the eigen value. (6)
   b) Write the Schrodinger wave equation for a free particle moving in three dimension and solve it for the eigen value and eigen function. Explain quantum mechanical degeneracy. (14)

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10. a) State the Great Orthogonallity theorem. Write any two properties of the representation. (8)
    b) Apply group theory to find out the symmetries of normal modes of vibration in BF_3 and find out which of item are IR and Raman active. (use of character table for D_{3h} is allowed) (12)

11. Set up Schröedinger equation for a simple harmonic oscillator and solve it for the eigen value and eigen function of the oscillator. What is meant by zero point energy of the oscillator. (20)