STELLA MARIS COLLEGE (AUTONOMOUS) CHENNAI-86
(For candidates admitted during the academic year 2019-20& thereafter)

SUBJECT CODE: 19CH/PC/QG24

M.Sc. DEGREE EXAMINATION, APRIL 2021
BRANCH IV - CHEMISTRY
SECOND SEMESTER

COURSE: MAJOR CORE
PAPER: QUANTUM CHEMISTRY AND GROUP THEORY
TIME: 90 minutes **MAX.MARKS:50**

SECTION-A

Answer all the questions **(11 x 1 = 11 Marks)**
I. Choose the correct answer:

1. Which among the following is a well-behaved wave function?

a) e^{x^2} b) e^{x} c) e^{-x} d) $e^{i\theta}$

2. The zero point energy of a particle in a one-dimensional box is:

a) 0 b) $h^2/8ma^2$ c)$3h^2/8ma^2$ d) $h^2/8m^2a^2$

3. The Hermite polynomial for n=1 is:

a) $4q^2$ b) 1 c) $2q^2$-2 d) 2q

4. Identify the molecule which does not possess a centre of symmetry

a) 1,4-dichloro-2,5-difluorobenzene b) dichloromethane c) staggered ferrocene
d) benzene

II Fill in the blanks:

5. The commutator for $[\widehat{Lx}, \widehat{Ly}]$ is _____

6. The conjugate of σ_{xz} in C_{2v} point group is _____

7. The symmetry of vibrational ground state of water molecule is _____

8. In the character table of C_{3v} point group, there are _____ one dimensional IRR and _____ two dimensional IRR.

III Answer in a line or two:

9. What is a rigid rotator with fixed axis?

10. Determine the position of the node on the r-axis for the 2s orbital of Hydrogen atom.

11. Prove that reflections through planes perpendicular to each other commute.

SECTION – B

Answer any three questions **(3x8=24 marks)**

12. Explain HMO treatment to 1,3-butadiene and arrive its wave function and energy.

13. a) Prove that the operators $\hat{A}$and $\hat{B}$ do not commute with each other for the function $\sin x$ and also prove that the commutator is a unit operator. **[4]**

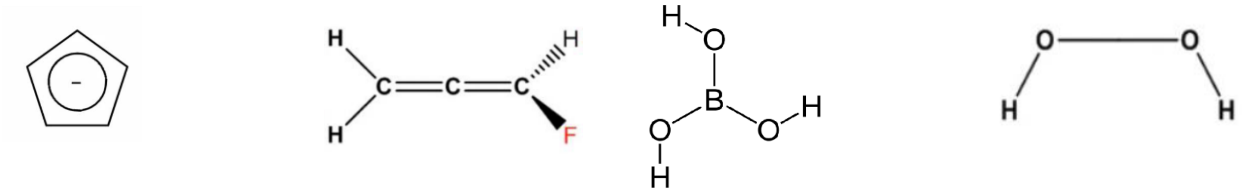
    b) The eigen value for a particle confined to move in a 3D box is $17h^2/8ma^2$. Determine the quantum numbers n_x, n_y, n_z and the degree of degeneracy. **[4]**

14. a) In the electronic spectrum of Formaldehyde, the π to π* transition is symmetry allowed, while the n to π* is symmetry forbidden. Explain the above statement using Group theory. **[6]**

    b) Explain the Symmetry operations: rotations and reflections in methane molecule. **[2]**

15. Identify the point groups of the following compounds and give their symmetry elements, order and number of classes.

a. b. c. d.



SECTION – C

Answer any One question **(1x15=15 marks)**

16. a) Prove that the angular momentum of rigid rotator is quantised. **[3]**

    b) Apply perturbation theory to helium atom and determine the first order perturbation correction energy for the ground state. **[8]**

    c) Write the character table of C_{2V} point group. **[4]**

17. a) Determine the position of the node on the r axis for the 3p orbital of the Be^{3+} ion. **[3]**

    b) Derive the ground state and excited state wave functions of He atom and prove that the electrons are paired in one excited state and parallel in three excited states. **[9]**

    c) Show that H_2O molecule belongs to abelian group whereas NH_3 molecule belongs to non-abelian group. **[3]**

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