C 4755 (Pages : 3) **Name..............................**

Reg. **No..........................**

SECOND SEMESTER M.Sc. DEGREE EXAMINATION, JUNE 2016

(CUCSS)

Chemistry

CH 2C 05—APPLICATIONS OF QUANTUM MECHANICS AND GROUP THEORY

(2015 Admissions)

Time : Three Hours Maximum 36 Weightage

Part A

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

1. State and explain independent particle model.
2. State and explain variation theorem.
3. Write Slater determinantal wave function for Li atom.
4. Distinguish between STO and GTO.
5. Arrange $0_2, O_2^+$ and O_2^- in the increasing order of stability. Justify your answer.
6. Write spectroscopic term symbol for C_2.
7. it- molecular orbitals of benzene are $a + 2\beta$, a + 0, a +13, $a - \beta$, $a - \beta$ and a – 2(3. Calculate the delocalization energy.
8. Draw Frost-Hückel mnemonic device for cyclo-prophenyl cation. Explain.
9. State Laporte selection rules for centro symmetric molecules.
10. You are given the integral $\int_{-a}^{+a} x^2 dx$ Check whether it is a vanishing integral or not.
11. Write projection operator $\hat{I}_{A_1}$ for C_{2_v}.
12. Distinguish between SALC and SAGO. State the conditions underwhich SALC becomes equal to SAGO.

(12 x 1 = 12 weightage)

Turn over

Part B

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

13. Find the ground state energy a particle confined to one-dimensional box of length 'a'. Use the trial function $\Phi = x(a - x)$.
14. Find the ground state energy of He by first order perturbation method.
15. Briefly explain Roothan's concept of basis functions.
16. State and explain non-crossing rule.
17. Apply HMO method to find the π- molecular orbitals and their energy values for allyl cation.
18. State mutual exclusion principle rationalise using group theory.
19. Find Raman and IR active vibrations of H_2O. Use C_{2v} character table :

C_{2v}	E	C_{2z}	σ_{vxz}	σ_{yz}		
A_1	**1**	**1**	**1**	**1**	z	x^2, y^2, z^2
A_2	**1**	**1**	**−1**	**−1**	Rz	xy
B_1	**1**	**−1**	**1**	**−1**	x, Ry	xz
B_2	**1**	**−1**	**−1**	**1**	y, Rx	yz

20. Find the symmetry species of molecular orbitals of HCHO (e_{2v}). Use C_{2v} character table given in Question No. 19.
21. Discuss bonding in H_2O using quantum mechanical approach.
22. Briefly discuss Hartree self consistent field method of solving many electron atoms.
23. State and explain Born—Oppenheimer approximation. Discuss its significance.
24. Find hybridized orbitals of B in BF_3. Use $D_{3}h$ character table :

D_{3h}	E	$2O_3$	C_2	$6h$	$2s_3$	3		
A_1	1	**1**	**1**	**1**	**1**	**1**		$x^2 + y^2, z^2$
A2	**1**	**1**	**−1**	**1**	**1**	−1	R_z	
	2	−1	0	2	−1	0	(x, y)	($x^2 - y^2$, xy)
A_1	1	1	1	−1	−1	−1		
A_2	1	1	−1	−1	−1	1		
	2	−1		−2	1	0	(Rx, Ry)	(xz, yz)

(8 x 2 =16 weightage)

Part C

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

25. Compare V.B. and M.O. method of bonding as applied to H_2. Which is found better ? Justify your answer.

26. Apply HMO method for n bonding in butadiene. Find the energy of it molecular orbitals.

27. Find IR and Raman active vibrations of ammonia. Use C_{3v} character table given below.

28. Find the ground state energy of H atom by variation method using the trial function $= e^{-ar}$.

C_{3v}	E	$2C_3$			
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	−1	R_z	
E	2	−1	0	(x, y) (R_x, R_y)	$(x^2 - y^2, xy)$ (xz, yz)

(2 x 4 = 8 weightage)