C 83711

Name.....

Reg. No.....

# SECOND SEMESTER M.Sc. DEGREE EXAMINATION, JUNE 2015

# (CUCSS)

### Chemistry

# CH 2C 04—THEORETICAL CHEMISTRY—II

## (2010 Admissions)

Time : Three Hours

Maximum : 36 Weightage

# Section A

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

- 1. Explain with examples :
  - (a) Abelian group. (b) Cyclic group.
- 2. Generate matrices for :
  - (a)  $C_3$ . (b)  $\sigma_{xy}$ .
- 3. Distinguish between degenerate and non-degenerate representation with examples.
- 4. Explain with example 'projection operator'.
- 5. Which of the following vanish on integration ? Illustrate :

a a 
$$(a) \mathbf{f} \mathbf{X}^2 dx.$$
 (b)  $\mathbf{f} \mathbf{x}^3 dx.$ 

- 6. Define normal mode of vibration.
- 7. State Laporte selection rules for centrosymmetric systems.
- 8. Which of the following molecules give microwave spectrum ? Why ?

(a) $\mathbf{CO}_{G}$ .	(b)	CH <sub>3</sub> Cl.
$ \subset C_2H_4.$	(d)	CH <sub>2</sub> Cl <sub>2</sub> .

- 9. Calculate the Doppler shift in frequency when radiation of frequency 10<sup>12</sup> MHz is absorbed by a sample moving with a velocity of 1 cm. 5<sup>-1</sup>.
- 10. Account for the decrease in spacing of lines in the pure rotation spectrum of HCl as J increases.

- 11. Find the number of vibrational quantum states in the ground electronic level of HCl. The an harmonic it constant is 0.017.
- 12. Explain terms 'isotropic polarizability' and 'Anisotropic polarizability'.
- 13. Define gyromagnetic ratio. Explain its significance.
- 14. What do you mean by 'COSY'. Explain.

# $(14 \times 1 = 14 \text{ weightage})$

#### Section B

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

- 15. Set up group multiplication table for  $C_{30}$  point group.
- 16. Derive  $c_{3u}$  character table.
- 17. Find IR and Raman active vibrations of  $H_2O$  which belongs to C2, point group

C2 <sub>1)</sub>	Е	C <sub>2z</sub>	ULL	уг		
A <sub>1</sub>	1	1	1	1	z	$x^2$ , $y^2$ , $z^2$
А <sub>2</sub> В1 В2	1	1 1 1	_1	_1	R_	xy
$B_1$	1	_ 1	1	-1	х, <b>R</b> <sub>,</sub>	xz
<b>B</b> <sub>2</sub>	1	_ 1	_1	1	y, R_	yz

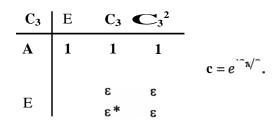
- 18. Find molecular Obitals in  $H_2O$  use  $C_{2\nu}$  character table in question No. 17.
- 19. How would you determine the bond lengths in COS using microwave spectroscopy ? Explain.
- 20. State and explain the selection rules for rotational Raman spectrum of polyatomic molecules.
- 21. What is 'Fortrat diagram' ? Explain its significance.
- 22. Briefly explain the principle of AES.
- 23. H atom shows EPR spectrum with a coupling constant of 50mT. Use McConnell equation to find the electron density around C atom in methyl radical which shows a coupling constant of 2.3 mT.
- 24. Briefly explain 'quadrapole relaxation'.

 $(7 \times 2 = 14 \text{ weightage})$ 

## Section C

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

- 25. Predict allowed electronic transactions in  $CH_2O$ . Use  $C_{zv}$  character table in question No. 17,
- 26. Find n molecular orbitals in  $(C_3H_3)$ . Use  $C_3$ . Character table :



- 27. How would you predict Raman activity using polarizability ellipsoid ? Discuss.
- 28. What are the drawbacks of field sweep method in NMR spectroscopy ? How are they overcome in FT NMR ? Discuss.

 $(2 \times 4 = 8 \text{ weightage})$