



(Pages : 2)

B – 4319

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, January 2017

Branch : Chemistry

CL/CA/CH 233 : PHYSICAL CHEMISTRY – III

(2013 Admission Onwards)

Time : 3 Hours

Max. Marks : 75

SECTION – A

Answer **any two** among **a, b** and **c** of **each** question. **Each** subquestion carries **2** marks. **(10×2=20 Marks)**

1. a) Explain the following terms :
 - I) Stationary point
 - II) Saddle point with reference to computational methods.
- b) Distinguish between polarized and differed basis set with examples.
- c) Write Z-matrix for NH_3 .
2. a) Distinguish between scalar coupling and dipolar coupling.
- b) State and explain Kramer's rules.
- c) Distinguish between ENDOR and ELDOR.
3. a) Arrange translational, rotational and vibrational partition function in the increasing order of magnitude. Justify your answer.
- b) What is Langevin's partition function ?
- c) Rotational motion does not contribute towards pressure of a gas. Justify the statement.
4. a) Spontaneous adsorption is always exothermic. Justify the statement.
- b) Write Harkin's Jura isotherm. Explain the terms.
- c) Write Langmuir adsorption isotherm in the linear form. What is the significance of the slope and intercept ?

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5. a) Explain the working of a Calomel electrode.
- b) How would you detect the end point in a titration by potentiometric method ? Explain.
- c) Explain the working of an atomizer in AAS.

SECTION - B

Answer either **a** or **b** of **each** question. **Each** question carries **5** marks. **(5×5=25 Marks)**

6. a) Explain the principle and applications of X-ray photoelectron spectroscopy.
- b) How is Doppler effect made use of in Mössbauer spectroscopy ? Explain.
7. a) What are the properties of Slater type of orbitals ? Discuss.
- b) What are the assumptions in Restricted Hartree Fock method ? Discuss.
8. a) How do you evaluate the equilibrium constant of a reaction from molecular data ? Discuss.
- b) How would you evaluate rotational partition function of molecular H_2 ? Discuss.
9. a) Derive Gibbs adsorption isotherm. How is it verified ? Discuss.
- b) Briefly explain microscopic methods of surface analysis.
10. a) Explain the working of glass electrode.
- b) 0.800 amperes of current is passed through an aqueous solution of $CuSO_4$ for 20 minutes. Calculate the amount of Cu deposited at the cathode.

SECTION - C

Answer **any three** questions. **Each** question carries **10** marks. **(3×10=30 Marks)**

11. Write a brief account of ab initio methods in computational chemistry.
 12. Discuss the theory and instrumentation in pulsed NMR.
 13. Briefly discuss Debye's theory of heat capacity of solids.
 14. Derive BET adsorption isotherm. Show that it approximates to Langmuir adsorption isotherm under limiting conditions. What is the limiting condition ?
 15. Discuss the principle and instrumentation in AAS.
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