



Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, January 2014

Branch : Chemistry

CH/CL/CA 233 : PHYSICAL CHEMISTRY III

(2009 Admission)

Time : 3 Hours

Max. Marks : 75

SECTION – A

Answer any two among 'a', 'b' and 'c' of each question. Each sub-question carries 2 marks.

1. a) Explain the following terms MM2, MM3, MP3.
b) What do you mean by HF/6-31 G* ?
c) Write Z-matrix for NH_3 .
2. a) How many lines do you expect in the EPR spectrum of $\dot{\text{N}}\text{H}_3$ (radical) ? Explain.
b) In AAS the source is made of the same element as the sample under analysis. Why ?
c) Write Wierl equation. Explain its significance.
3. a) 3 particles show a total energy of 3ε . The allowed quantum states are 0, 1ε , 2ε and 3ε . What are the possible macrostates according to Fermi Dirac statistics ? Explain.
b) State and explain Dulong Petit's law.
c) Calculate the heat capacity of demand at 1.86 K. Its characteristic temperature is 1860K.
4. a) Write Gibbs adsorption isotherm. How is it verified ?
b) Define isosteric heat of adsorption.
c) Define surface pressure. How is it measured ?
5. a) Write electrode reaction of a calomel electrode. Explain.
b) What is coulometric titration ? Explain.
c) Define half wave potential. Explain its significance.

(10×2=20 Marks)

P.T.O.



SECTION – B

Answer either 'a' or 'b' of each question. Each question carries 5 marks.

6. a) Write a brief account of the Gaussian input file.
b) Compare ROHF and URHF methods.
 7. a) What is Kramer's degeneracy ? Discuss.
b) How would you determine $g_{||}$ and $g_{\perp}$? Explain.
 8. a) Show that fermions and bosons follow Maxwell Boltzman statistics under dilute system condition.
b) Derive Einstein's heat capacity equation for solids.
 9. a) What are the methods for the determination of surface area of a solid ? Discuss.
b) What are the steps in surface catalysed reaction ? Discuss.
 10. a) Explain the working of a glass electrode.
b) How do you detect the end point in potentiometric titration ? Explain.
- (5×5=25 Marks)**

SECTION – C

Answer any three questions. Each question carries 10 marks.

11. Write a brief account of the semi empirical methods in computational chemistry.
 12. Discuss the theory and instrumentation in AAS.
 13. Apply Fermi Dirac statistics for electrons in metals. Discuss.
 14. What are the assumptions in BET adsorption isotherm ? Derive BET adsorption isotherm. Express the isotherm in linear form.
 15. Write a brief account of the various voltammetric techniques.
- (3×10=30 Marks)**
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