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8482

Reg. No. :

Name :

Third Semester M.Sc. Degree Examination, February 2015

Branch : Chemistry

CH/CL/CA 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) What do you mean by contracted Gaussian ? Explain.
b) Explain with example 'Open shell' approach in computational chemistry.
c) Write Z-matrix for H_2CO .
2. a) Define gyromagnetic ratio. Explain its significance.
b) How many lines do you expect in the ESR spectrum of ND_3 radical ? Justify your answer.
c) How would you distinguish between XPS and AES lines in the spectrum ?
3. a) Calculate C_v for NH_3 using equipartition principle.
b) State and explain Kopp's law.
c) Calculate the characteristic temperature of HCl . The vibrational frequency is 3000 cm^{-1} .
4. a) Explain the terms KLL and KLM with reference to photo electron spectroscopy.
b) Define isosteric heat of adsorption.
c) Unimolecular surface catalysed gas phase reactions follow first order kinetics at low pressures and zero order kinetics at high pressures. Justify the statement.

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5. a) During the titration of Fe^{2+} against potassium dichromate using diphenylamine as indicator orthophosphoric acid is added. Why ?
b) What is coulometric titration ?
c) In AAS, radiation from the same element under examination is used as source. Why ?

SECTION – B

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

6. a) What are the methods for finding 'saddle point' ? Discuss.
b) What are the guidelines for choosing basis functions ? Discuss.
7. a) Briefly explain 2-dimensional NMR experiment.
b) What is zero field splitting ? Discuss.
8. a) Calculate rotational partition function of CO at 25°C. The bond length is 1.13 Å.
b) Calculate the heat capacity of diamond at 1000 K. The characteristic temperature is 1860 K.
9. a) Briefly discuss Langmuir-Henshelwood model of bimolecular surface catalysed reaction.
b) Derive Langmuir adsorption isotherm from statistical point of view.
10. a) Briefly explain the working of a hollow cathode lamp.
b) Discuss the principle and applications of cyclic voltammetry.

SECTION – C

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

11. Write a brief account of the semi-empirical methods in computational chemistry.
12. Discuss the principle and applications of NQR spectroscopy.
13. Write Virial equation of state of a real gas. Evaluate the first Virial coefficient.
14. Explain the term 'low energy electron diffraction'. Discuss its application in surface analysis.
15. Discuss the theory and applications of polarographic method of analysis.
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