

Reg. No. : .....Name: ..... **P231**

**M. Sc. DEGREE END SEMESTER EXAMINATION APRIL 2016**  
**SEMESTER - 2: PURE CHEMISTRY/ APPLIED CHEMISTRY**  
**COURSE: P2CHET07-P2CPHT07: CHEMICAL BONDING AND COMPUTATIONAL**  
**CHEMISTRY**

*(Common for Regular- 2015 Admission /Supplementary-2014 Admission)*

Time: Three Hours

Maximum Marks: 75

**SECTION A**

(Answer **any ten** questions, each question carries 2 marks)

1. Explain Hellmann-Feynman theorem.
2. Mention the physical significance of stationary points.
3. What are Gaussian Type Orbitals (GTOs)? Mention their advantages
4. What are Slater determinants?
5. Explain non-crossing rule by taking a heteronuclear diatomic molecule.
6. What are projection operators? Explain its importance.
7. What do you mean by basis set approximation?
8. What is Hartree-Fock limit?
9. What do you mean by configuration- interaction?
10. What is hybrid functional?
11. Differentiate between local and global minima.
12. What are the important features of AMBER?
13. State and explain Koopmans' theorem. (2 × 10 = 20)

**SECTION B**

(Answer **any five** questions, each question carries 5 marks)

14. Prove variation theorem.
15. Calculate the free-valence indices at all the carbon atoms in allyl cation.
16. State and explain Hohenberg-Kohn theorems.
17. Write a note on Roothan's concept of basis functional.
18. Using group theoretical considerations obtain the hybrid orbitals in BF<sub>3</sub>.
19. What are basis sets? Discuss minimal and split valence basis set.
20. What is Z-matrix? Obtain the Z-matrix for staggered ethane molecule.
21. What is model chemistry? Explain the notations [MP2/6-31G(d,p); HF/6-31G]

**P231**

**SECTION C**

(Answer any **two** questions, each question carries 15 marks)

22. Explain the basic principle of computation methods based on Density Functional Theory (DFT).
23. Write a note on perturbation method with reference to first order correlation to energy and wave function.
24. Apply Hückel Molecular Orbital (HMO) theory to butadiene and calculate its charge distribution.
25. Give the general format of GAMESS input file. How it is similar to firefly?  
(2 × 15 = 30)

\*\*\*\*\*