Roll No.....

P. G. Diploma in Chemo-informatics
Annual Examination – 2010
Computational Chemistry
PGDC – 106

Time allowed : 2½ Hours **Max Marks:70**

Note: This paper is divided into three sections. Attempt all questions from Section – A, any six questions from section – B and any three questions from section - C

Section – A

Answer appropriately. Each question caries (1) marks [1 x 10]

1. Molecular Mechanics is the process of finding a _____ of an empirical potential function.
2. Molecular Dynamics and Monte Carlo are based on principles of _____.
3. Hartree – Fock Theory was developed to solve the _____ _____ _____.
4. A Z – matrix is used to define _____ between atoms in a molecule.
5. A potential energy surface represents the potential energy of a molecule as a function of its _____.
6. D I I S stands for _____ _____ _____ _____.
7. Beta Glucan is extracted from the cell walls of _____ _____.
8. _____ is a software that performs Monte Carlo statistical mechanics simulations.
9. The Y – component of angular momentum, L, is Ly = ZPx – XPz (True/False)
10. The ware function does not completely specify the state of a quantum mechanical system.

Section – B

Attempt any **six** questions. All questions carry equal marks. [6 x 5 = 30]

1. Give the principles of molecular mechanics methods, and the range of its applicability.
2. Explain what do you understand by Slater Determinants.
3. Build up the Z- matrix for the following molecules (any two)
   a) Water b) Ammonia c) Ethylene d) Acetylene
4. What types of properties are predicted by the electronic wave function.
5. Give the mathematics of Direct Inversion of Iterative Subspaces.
6. Describe the photoelectric effect.
7. Describe Born-Oppenheimer approximations.
8. Explain the postulates of Quantum Mechanics.

Section – C

Attempt any **THREE** questions. All questions carry equal marks. [3 x 10 = 30]

1. Write a concise note on Beta Glucan Technologies.
2. Explain what you understand of Linear Vector spaces in quantum mechanics.
3. Describe Monte Carlo Method.
4. Write a note on Rydberg Transitions.
5. Write notes on the following
   a) Geometry Optimization. b) Potential Energy Surfaces (PES) c) Wave particle duality.
6. What are the basic principles of molecular mechanics? Explain force field.