CODE NO: RR 412 310

2005 JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY

IV B.TECH I SEMESTER REGULAR EXAMINATIONS
MOLECULAR MODELLING AND DRUG DESIGN
(BIO-TECHNOLOGY)

NOVEMBER 2005

TIME: 3 HOURS
MAX MARKS: 80

Answer any FIVE Questions
All Questions carry equal marks

1. What is central multipole expansion? How is it used to describe molecules?

2. What are London forces? Describe how they are treated in molecular modeling.

3. Give a brief account of molecular dynamics method of molecular simulation.

4. What is a block method in a molecular simulation program? Describe its use and importance in improving the molecular simulation programme.

5. (a) Describe the use of Lennard - Jones potential in calculation of force between two atoms.

(b) How this force calculation is implemented using loops in molecular dynamics simulation?

6. Describe the use of SHAKE method with Verlet algorithm.

7. Explain the following :

(a) Markov chain

(b) transition matrix

(c) stochastic matrix

(d) Boltzman factor.

8. Describe how Monte Carlo Simulation methods can be used for simulations of atomic and small molecular systems.