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. Describe briefly the importance of electrostatic interactions in modeling a molecule.

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

3. Explain the following :

(a) expectation value

(b) time average

(c) probability density

(d) deterministic method.

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

5. What are finite difference methods? Describe any one such method used in molecular dynamics simulation.

6. Describe in detail SHAKE procedure of molecular dynamics.

7. Derive an expression for canonical partition function of an ideal gas.

8. What are polymers? What are different types of polymers? What are the different types of models used in simulation of polymers? How do they differ in complexity of simulation?