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.
[16]

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

[6+6+4]

3. Explain the following :

(a) expectation value
(b) time average
(c) probability density
(d) deterministic method.

[4+4+4+4]

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

[10+6]

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

[6+10]

6. Describe in detail SHAKE procedure of molecular dynamics.

[8+8]

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

[8+8]

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?

[8+8]