Code No: RR412312 **Set No. 1**

**IV B.Tech I Semester Regular Examinations, November 2005**
**MOLECULAR MODELLING AND DRUG DESIGN**
**(Bio-Technology)**

**Time: 3 hours** **Max Marks: 80**

**Answer any FIVE Questions**
**All Questions carry equal marks**

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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+10]
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. [4+12]
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. [16]
7. Derive an expression for canonical partition function of an ideal gas. [16]
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? [3+4+4+5]

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Code No: RR412312 **Set No. 2**

**IV B.Tech I Semester Regular Examinations, November 2005**
**MOLECULAR MODELLING AND DRUG DESIGN**
**(Bio-Technology)**

**Time: 3 hours** **Max Marks: 80**

**Answer any FIVE Questions**
**All Questions carry equal marks**

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1. What is polarization? What is its importance in molecular modeling? [6+10]
2. Explain the following :
   (a) simple water models
   (b) flexible water models. [8+8]
3. What is a computer simulation? How does it help in understanding molecular systems? What are the two basic types of molecular simulations? How do they differ from each other? [4+4+4+4]
4. Describe how various properties are monitored during the equilibrium phase of a computer simulation of a molecular system. [16]
5. Describe very briefly any four integration methods used in molecular dynamics simulation of molecules with continuous potentials. [16]
6. What are time correlation coefficients? Describe briefly how molecular dynamics simulation can be used to calculate them. [4+12]
7. Explain the following :
   (a) Monte Carlo method
   (b) Metropolis method
   (c) Markov chain
   (d) random number generator. [4+4+4+4]
8. Explain the following :
   (a) cut off region
   (b) preferential sampling procedure
   (c) force-bias Monte Carlo method
   (d) Smart Monte Carlo method. [4+4+4+4]

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Code No: RR412312 **Set No. 3**

**IV B.Tech I Semester Regular Examinations, November 2005**
**MOLECULAR MODELLING AND DRUG DESIGN**
**(Bio-Technology)**

**Time: 3 hours** **Max Marks: 80**

**Answer any FIVE Questions**
**All Questions carry equal marks**

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1. What are the different functional forms used to analyze various out-of-plane bending terms. [4+12]
2. Describe briefly how different types of Vander Waals interactions between atoms are described in molecular modeling. [4+12]
3. Explain in brief the concept of boundaries in molecular systems. [16]
4. What is a block method in a molecular simulation program? Describe its use and importance in improving the molecular simulation programme. [4+12]
5. (a) Describe Newton's Laws of motion
   (b) Describe the three types of situations in molecular dynamics to which Newton's laws of motion may be applied.
   (c) Explain the hard-sphere model of molecular dynamics
   (d) Explain the square well potential method of molecular dynamics. [4+4+4+4]
6. Explain the following :
   (a) **SHAKE** procedure
   (b) **RATTLE** method
   (c) Logrange multiplier
   (d) constraints and restraints. [4+4+4+4]
7. What is the difference between Metropolis method and other Monte Carlo methods in calculating thermodynamic properties. Explain the significance of Metropolis method. [8+8]
8. Explain the "configurational bias Monte Carlo" (CBMC) method. [16]

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Code No: RR412312 **Set No. 4**

**IV B.Tech I Semester Regular Examinations, November 2005**
**MOLECULAR MODELLING AND DRUG DESIGN**
**(Bio-Technology)**

**Time: 3 hours** **Max Marks: 80**

**Answer any FIVE Questions**
**All Questions carry equal marks**

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1. What is central multipole expansion? How is it used to describe molecules?[4+12]
2. What are London forces? Describe how they are treated in molecular modeling. [6+10]
3. Give a brief account of molecular dynamics method of molecular simulation. [16]
4. What is a block method in a molecular simulation program? Describe its use and importance in improving the molecular simulation programme. [4+12]
5. (a) Describe the use of Lennard - Jones potential in calculation of force between two atoms. [4+4]
   (b) How this force calculation is implemented using loops in molecular dynamics simulation? [8]
6. Describe the use of **SHAKE** method with Verlet algorithm. [16]
7. Explain the following :
   (a) Markov chain
   (b) transition matrix
   (c) stochastic matrix
   (d) Boltzman factor. [4+4+4+4]
8. Describe how Monte Carlo Simulation methods can be used for simulations of atomic and small molecular systems. [8+8]

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