

Avinashilingam Institute for Home Science and Higher Education for Women  
Coimbatore – 641 043

Master's Degree Examination – November 2017  
III Semester

Class: II P.G  
Major: Physics

Time : 3 hrs  
Max Marks : 60

Interdisciplinary Course - II  
12MBII02 Molecular Modelling Techniques

PART- A

Choose the Correct Answer

(10 X ½ = 05)

1. What view of a molecule gives the best indication of its shape?  
(A). Ball and stick model (B). Skeletal model  
(C). Hydrogen bonding surface (D). Van der Waals surface
2. What colour is normally used for oxygen atoms in molecular models?  
(A). Blue (B). Black  
(C). Red (D). Orange
3. Molecules that have to adopt an \_\_\_\_\_ conformation in order to bind should be rejected.  
(A). unstable (B). stable  
(C). both A and B (D). None of the above
4. \_\_\_\_\_ structures are useful in determining an active conformation.  
(A). Non- Cyclic (B). Cyclic  
(C). Rectangle (D). Triangle
5. \_\_\_\_\_ is where a molecular ligand is fitted into its binding site by molecular modelling.  
(A). nitrifying (B). nitrification  
(C). triggering (D). Docking
6. Semi-empirical quantum chemistry methods are based on the \_\_\_\_\_ formalism  
(A). Carl copper (B). Mendelian  
(C). Hartree-Fock (D). Albert Einstein
7. What name is given to a molecule that bonds to the active site of an enzyme and deactivates it?  
(A). An enzyme inhibitor (B). substrate activator  
(C). active site (D). None of the above
8. What molecule normally bonds to the active site of a neuraminadase molecule?  
(A). niacin (B). ascorbic acid  
(C). cyanocobalamine (D). Sialic acid
9. Nelder-Mead method is also called as  
(A). downhill simplex method (B). amoeba method  
(C). Both A and B (D). None of the above
10. Fibonacci search and golden-section search were discovered by  
(A). Robert Einstein (B). Kalvin  
(C). Newton (D). Kiefer

**PART – B**

**(5 X 4 = 20)**

**Answer all the questions**

**Answer should not exceed 200 words or one pages**

11. (a). Describe the internal energy of molecular modelling.

(or)

(b). Elucidate the types of movement.

12. (a). Discuss the Schrodinger equation.

(or)

(b). Explain the Born-Oppenheimer approximation.

13. (a). Write a note on basis of sets.

(or)

(b). Discuss the semi-empirical method.

14. (a). Write a principles of molecular mechanics.

(or)

(b). Illustrate about bonded interactions of molecular mechanics.

15. (a). Describe the golden section search.

(or)

(b). Write a note on downhill simplex method.

**PART – C**

**(3 X 7 = 35)**

**Answer any three questions**

**Answer should not exceed 600 words or three pages**

16. (a). Give a detail note on Ramachadran plot.

(or)

(b). Explain the potential energy surfaces of molecular modelling.

17. (a). Describe the poly electronic atoms.

(or)

(b). Explain the Hartree-fock approximation.

18. (a). Explain the potential energy calculation using semi empirical methods.

(or)

(b). Write an account on Roothaan-Hall approach.

19. (a). Enumerate the general features of molecular mechanics forces fields.

(or)

(b). Describe the modeling macro molecules.

20. (a). Explain the Newton and Quasi-Newton method.

(or)

(b). Elucidate the conjugate gradient method of first order derivatives methods.

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