Roll No. | | | | | | | | | | | | |

Total No. of Pages : 02

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M.Sc.(Chemistry) (2015 to 2017) (Sem.–3)

COMPUTATIONAL SKILLS AND SIMULATIONS IN CHEMISTRY

Subject Code : MSCH-303

M.Code : 72621

Time : 3 Hrs. Max. Marks : 100

INSTRUCTION TO CANDIDATES :

1. **Attempt any FIVE questions, including compulsory Question No.1, ONE question from EACH UNIT.**

1. Explain briefly : 10×2=20

a) OPLS force field

b) Global energy minima

c) Rigid docking

d) Softwares for quantum energy calculation

e) Cartesian stochastic (or random kick) method

f) INDO

g) Molecular mechanics

h) MP method

i) Gas phase thermodynamics

j) Intermolecular forces

UNIT-I

2. Describe fundamental principles applied to generate most stable conformation in computer screen. 20

3. Describe principle and chemical applications of Monte Carlo method of molecular simulation. 20

UNIT-II

4. Describe ab-initio quantum chemical methods for calculating quantum energy of molecules. What are the advantages of these over semi-empirical methods? 20

5. Write short notes on :

   a) Basis set of ab-initio theory 10

   b) Application of Hartree-Fock theory 10

UNIT-III

6. Give principle and applications of Coupled cluster theory. 20

7. What is CI method of electron correlation? Give its advantages over the other methods. 20

UNIT-IV

8. Give a description on the methods to calculate vibrational frequencies. 20

9. What is DFT? What are its applications? 20

NOTE : Disclosure of Identity by writing Mobile No. or Making of passing request on any page of Answer Sheet will lead to UMC against the Student.