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

Paper ID : [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.**

Q1 Explain briefly :

a) Docking.

b) DREIDING Force Field.

c) Trajectories.

d) The simplex search algorithm of energy minimization.

e) Semi-empirical quantum mechanical calculation.

f) Hartree-Fock approximation.

g) AMI quantum model.

h) Coulomb electronic correlation.

i) Slater Type Orbitals.

j) Global energy minima.

UNIT-I

Q2 a. What are the advantages and limitations of Force field methods? (10)

b. Enumerate important force fields comment on their specific uses. (10)

Q3 a. Describe first derivative method of energy minimization. (10)

b. Describe the biochemical applications of Monte Carlo simulations. (10)

UNIT-II

Q4 a. What are the advantages and limitations of ab initio method? (5)

b. What are the neglect of diatomic differential overlap (NDDO) semi-empirical methods? Comment on General Performance of NDDO Models. (15)

Q5 a. What are Key Technical and Practical Points of Hartree-Fock Theory? (8)

b. Describe Contracted Basis Sets. (12)

UNIT-III

Q6 a. What are Dynamical and Non-dynamical Electron Correlation in molecular orbital theory? Discuss about Excited Slater Determinants. (15)

b. Describe Limitations of Multi-Configuration Self-Consistent Field (MCSCF) method. (5)

Q7 Name three main methods for calculating electron correlation. Describe any one in detail. (20)

UNIT-IV

Q8 Explain Kohn-Sham concept of DFT. What are its advantages and limitations? (20)

Q9 Give comprehensive account of computational modelling of CX stretching frequencies for CH_3X molecules using various quantum mechanical calculations. (20)