

- (b) Enlist the steps involved in the linear regression analysis.
- (c) Describe the term Chemical space. How can you access to chemical databases? (5×3)

(1000)

[This question paper contains 4 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 6056

H

Unique Paper Code : 2174001209

Name of the Paper : GE : Molecular Modelling,
Artificial Intelligence and
Machine Learning

Name of the Course : B.Sc. (H) / B.Sc. (Prog.)

Semester : II

Duration : 2 Hours

Maximum Marks : 60

Instructions for Candidates

1. Write your Roll No. on the top immediately on receipt of this question paper.
2. Attempt any **two questions each from Section A and Section B.**
3. **All** questions carry equal marks.
4. **Answer** four questions in all.

SECTION A

1. Write short notes on any **three** of the following.

(5×3)

P.T.O.

- (i) Molecular mechanics
 - (ii) Ab Initio Methods
 - (iii) Saddle point
 - (iv) Binding energy
2. (a) How many dimensions are needed to depict the potential energy diagram of the following molecules: H_2O , CO_2 , CH_4 ?
- (b) List any three molecular mechanics force fields and discuss their applications.
- (c) What do you understand by energy minimization? Explain steepest descent method for locating minima. (5×3)
3. (a) Give an expression for a 'molecular mechanics' potential energy function. Very briefly, explain each term.
- (b) The potential energy surface of HOF is a hypersurface. Comment.

- (c) Discuss the application of Schrödinger equation to tools of computational chemistry. (5×3)

SECTION B

4. (a) Discuss briefly how Artificial Intelligence can be used in the field of Chemistry.
- (b) Explain various steps that are involved in Drug Discovery.
- (c) What is dimensionality reduction? Explain any two methods of dimensionality reduction. (5×3)
5. (a) Explain physiochemical parameters of QSAR method with suitable examples.
- (b) What is genetic algorithm? Explain various types of genetic algorithm.
- (c) What are SMILES codes in computational chemistry? Explain any two examples. (5×3)
6. (a) Differentiate between Traditional and Algorithm search.