

[This question paper contains 2 printed pages.]

Your Roll No.....

Sr. No. of Question Paper : 7860

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Unique Paper Code : 2173540022

Name of the Paper : DSE- MACHINE LEARNING AND ARTIFICIAL
INTELLIGENCE IN CHEMISTRY

Name of the Course : **B.Sc. (Prog.)**

Semester : VIII, DSE

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 4 questions in all.
3. Question No. 1 is Compulsory.
4. All question Carry equal marks.

1. Attempt any **five** :

(A) What is the role of Artificial Intelligence (AI) in modern chemistry?

(B) Write some applications of AI in chemical research.

(C) What type of data is commonly used in ML models for chemistry?

(D) What is overfitting in ML models?

(E) How does AI help in predicting chemical reactions?

(F) What are the limitations of AI in chemistry research? (5×3)

P.T.O.

2. (A) Explain the concepts of Artificial Intelligence (AI) and Machine Learning (ML). Highlight differences between them.
- (B) What is model evaluation? Describe commonly used evaluation metrics in Machine Learning.
- (C) Describe how ML/AI can be used to predict molecular properties. Give suitable examples. (3×5)
3. (A) Explain model selection in Machine Learning. What factors should be considered while choosing a model?
- (B) Define a random variable. Distinguish between discrete and continuous random variables with examples.
- (C) What is Kernel Ridge Regression? How does it differ from Linear Regression?
4. (A) What is data pre-processing? Discuss its importance and common techniques used in ML.
- (C) Explain matrix multiplication with an example. What are the conditions for two matrices to be multiplied?
- (C) Differentiate between supervised and unsupervised learning with suitable examples.
5. (A) Discuss the role of AI/ML in molecular design and discovery of new compounds.
- (B) What is binding affinity prediction? Explain its importance in drug discovery.
- (C) Explain the concept of backpropagation in neural networks qualitative explanation). (3×5)