Reg. No. : ....

Code No.: 5425   Sub. Code: ZCHM 44

M.Sc. (CBCS) DEGREE EXAMINATION, APRIL 2023.

Fourth Semester

Chemistry – Core

SELECTED TOPICS IN CHEMISTRY

(For those who joined in July 2021 onwards)

Time : Three hours   Maximum : 75 marks

PART A — (10 × 1 = 10 marks)

Answer ALL questions.

Choose the correct answer :

1.   What are the three types of calculations commonly performed in computational chemistry

   (a) Energy prediction, geometry optimization, frequency prediction

   (b) Energy prediction, molecular dynamics, protein folding

   (c) NMR spectroscopy, IR spectroscopy, UV-Vis spectroscopy

   (d) None of the above

2.   Which of the following basis sets includes additional functions to account for diffuse electron density?

   (a) Minimal basis sets

   (b) Split valence basis sets

   (c) Polarized basis sets

   (d) Diffuse basis sets

3.   What is the purpose of an electrochemical cell in corrosion?

   (a) To generate electricity from corrosion

   (b) To measure the rate of corrosion

   (c) To prevent corrosion

   (d) To promote corrosion

4.   What is the purpose of a reference electrode in electrochemical corrosion measurement?

   (a) To measure the potential difference between the metal being corroded and the environment

   (b) To provide a standard potential against which other potentials can be measured

   (c) To measure the rate of corrosion

   (d) To prevent corrosion

5.   Which of the following is a technique used to extract and concentrate analytes from a liquid sample onto a small sorbent material?

   (a) Solid-phase extraction

   (b) Solvent extraction

   (c) Thin-layer chromatography

   (d) Gas chromatography

6.   Which of the following is a carrier gas commonly used in gas chromatography?

   (a) Nitrogen   (b) Water

   (c) Methanol   (d) Ethanol

7.   Which of the following is a primary type of transducer?

   (a) Thermistor   (b) Strain gauge

   (c) Thermocouple   (d) None of the above

8.   Which of the following is an example of a passive transducer?

   (a) Thermistor   (b) Photodiode

   (c) Strain gauge   (d) None of the above

9.   What is the most commonly used type of MRI contrasting agent?

   (a) Gadolinium-based agents

   (b) Manganese-based agents

   (c) Fe(III)-based agents

   (d) Fe(II)-based agents

10.   Which of the following is a merit of Fe(II)-based MRI contrasting agents?

   (a) High toxicity

   (b) Long half-life

   (c) High efficacy

   (d) Difficult elimination from the body

PART B — (5 × 5 = 25 marks)

Answer ALL questions, choosing either (a) or (b).
Each answer should not exceed 250 words.

11.   (a) What are the types of calculations commonly performed in computational chemistry? What information do they provide?

   Or

   (b) What are the different computational methods used in computational chemistry? How do they differ?

12. (a) What is corrosion inhibition and how is it classified? Give mechanism of inhibitor action in acidic medium.

Or

(b) What are potentiodynamic polarization monitoring and impedance monitoring?

13. (a) What is ion exchange chromatography? Explain it.

Or

(b) What are the basic components of a high-performance liquid chromatography (HPLC) system and how are they used in separation techniques?

14. (a) What is a chemical sensors? Give an examples.

Or

(b) What is an enzyme-based biosensors? Give an examples.

15. (a) What are the different types of nuclear imaging, and how do they differ?

Or

(b) How were MRI contrasting agents developed, and what are the different types of contrasting agents?

PART C — (5 × 8 = 40 marks)

Answer ALL questions, choosing either (a) or (b)
Each answer should not exceed 600 words.

16. (a) (i) What are Ab initio methods, and how do they differ from other computational methods in computational chemistry?

(ii) Explain the semi-empirical methods used in computational chemistry and their applications.

Or

(b) Explain the different types of basis sets commonly used in computational chemistry and their relative strengths and weaknesses.

17. (a) What is corrosion? What are the different types of corrosion? What are the electrochemical principles of corrosion and how do they relate to corrosion prevention?

Or

(b) How do pH, environmental factors such as temperature, humidity, and pollutants which affect the corrosion?

18. (a) How is micro extraction used in environmental monitoring?

Or

(b) What is solid-phase nano extraction (SPNE)?

19. (a) (i) What is a sensor, and how do they work?

(ii) What are transducers, and how do they relate to sensors?

Or

(b) (i) What is an enzyme-based biosensor, and how does it work?

(ii) What are some potential applications of sensors and biosensors?

20. (a) (i) What are the different types of MRI contrasting agents, and how were they developed?

(ii) What are the advantages and disadvantages of Gadolinium-based MRI contrasting agents?

Or

(b) (i) What are targeted and organ-specific contrast agents, and how do they improve medical imaging?

(ii) How are radio isotopic imaging agents used in nuclear imaging, and what are their requirements for effective use?

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