



M.Sc. I Semester Degree Examination, April/May - 2024

Skill Enhancement Courses (SEC)

INDUSTRIAL CHEMISTRY

SEC I SET B : Computational Chemistry

(NEP)

Time : 1 Hour

Maximum Marks : 30

1. Constants for Henry's law are computed from :
(A) Vapour pressure (B) $\log p$
(C) Group additivity methods (D) All of these

2. _____ methods have yielded the most accurate results of boiling point & melting point.
(A) QSPR (B) Rule based system
(C) Optimization (D) Time dependent methods

3. The _____ computations that are derived directly from theoretical principles with no inclusion of experimental data.
(A) Semi empirical methods (B) empirical methods
(C) graphics (D) Ab initio methods

4. In terms of solubility, database techniques are very accurate for _____.
(A) Inorganic compounds (B) Organic compounds
(C) Electron deficient compounds (D) Highly reactive compounds

5. Colligative properties, which are due to the interaction between molecules, can be computed more reliably with methods based on _____.
(A) thermodynamics
(B) statistical mechanics
(C) structure-activity relationships
(D) all of these



6. A helium atom is moving with a velocity $v = 20i - 15j$ m/s. What is its speed ?
 (A) 10 m/s (B) 25 m/s (C) 15 m/s (D) 5 m/s

7. Find the multiplication of vectors.

$$2 \begin{bmatrix} -1 & 2 \\ 0 & 4 \end{bmatrix}$$

(A) $\begin{bmatrix} -2 & 4 \\ 0 & 8 \end{bmatrix}$ (B) $\begin{bmatrix} -1 & 4 \\ 0 & 8 \end{bmatrix}$ (C) $\begin{bmatrix} -2 & 4 \\ 2 & 8 \end{bmatrix}$ (D) $\begin{bmatrix} -2 & 4 \\ 2 & 4 \end{bmatrix}$

8. An Argon atom is moving with a velocity v of $i + 7j + 4k$ m/s. What is its speed ?

(A) $\sqrt{65}$ (B) $\sqrt{55}$ (C) $\sqrt{45}$ (D) $\sqrt{66}$

9. Find the multiplication of vectors.

$$\frac{1}{2} \begin{bmatrix} 2 & 2 \\ 4 & 4 \end{bmatrix}$$

(A) $\begin{bmatrix} 2 & 2 \\ 4 & 4 \end{bmatrix}$ (B) $\begin{bmatrix} 1 & 1 \\ 4 & 4 \end{bmatrix}$ (C) $\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}$ (D) $\begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix}$

10. An Neon atom is moving with a velocity v of $i + 6j + 3k$ m/s. What is its speed ?

(A) $\sqrt{65}$ (B) $\sqrt{55}$ (C) $\sqrt{45}$ (D) none of these

11. Find the product of the two matrices $\begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 2 & 1 \end{bmatrix}$

(A) $\begin{bmatrix} 3 & 2 \\ 4 & 3 \end{bmatrix}$ (B) $\begin{bmatrix} 2 & 2 \\ 4 & 4 \end{bmatrix}$ (C) $\begin{bmatrix} 3 & 1 \\ 8 & 3 \end{bmatrix}$ (D) $\begin{bmatrix} 2 & 1 \\ 3 & 4 \end{bmatrix}$

12. Which one of the following is 3×3 identity matrix ?

(A) $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ (B) $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$ (C) $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ (D) none of these



13. For the matrix X find X^T where $X = \begin{bmatrix} 3 & 4 \\ 8 & 9 \end{bmatrix}$

(A) $\begin{bmatrix} 3 & 4 \\ 8 & 9 \end{bmatrix}$

(B) $\begin{bmatrix} 9 & -4 \\ -8 & 3 \end{bmatrix}$

(C) $\begin{bmatrix} 3 & 8 \\ 8 & 9 \end{bmatrix}$

(D) $\begin{bmatrix} 3 & 8 \\ 4 & 9 \end{bmatrix}$

14. Find the determinant of the matrix A

$$A = \begin{pmatrix} 1 & -4 \\ 2 & 5 \end{pmatrix}$$

(A) 25

(B) 13

(C) 20

(D) 15

15. Find the inverse A^{-1} of the matrix A.

$$A = \begin{pmatrix} 1 & -4 \\ 2 & 5 \end{pmatrix}$$

(A) $\begin{bmatrix} \frac{5}{13} & \frac{4}{13} \\ \frac{-2}{13} & \frac{1}{13} \end{bmatrix}$

(B) $\begin{bmatrix} \frac{1}{13} & \frac{4}{13} \\ \frac{-2}{13} & \frac{5}{13} \end{bmatrix}$

(C) $\begin{bmatrix} \frac{5}{13} & \frac{-4}{13} \\ \frac{2}{13} & \frac{1}{13} \end{bmatrix}$

(D) $\begin{bmatrix} \frac{-5}{13} & \frac{4}{13} \\ \frac{-2}{13} & \frac{-1}{13} \end{bmatrix}$

16. Differentiate $y = \frac{x}{e^{2x}}$

(A) $e^{-2x}(1-2x)$

(B) $e^{-2x}(1-x)$

(C) $e^{-x}(1-2x)$

(D) $e^{-2x}(1-5x)$

17. The ideal gas equation is $pV = nRT$. Find $\left(\frac{\partial V}{\partial T}\right)_P$.

(A) $\frac{nR}{V}$

(B) $\frac{pR}{V}$

(C) $\frac{nR}{P}$

(D) $\frac{nR}{T}$

18. Find the integrals of $x(x+3)$.

(A) $\frac{x^3}{3} + C$

(B) $\frac{x^3}{3} + 3x + C$

(C) $3\frac{x^3}{3} + C$

(D) $\frac{x^3}{3} + 3\frac{x^2}{2} + C$



19. Find $\int_0^{\pi} \sin(x) dx$

- (A) 1 (B) 0 (C) 2 (D) 4

20. If $\frac{dy}{dx} = 2x$ then use the method of separation of variables to integrate with respect to x .

- (A) $x^3 + C$ (B) $x^4 + C$ (C) $x^2 + C$ (D) none of these

21. $\int (3x^2 + 2x + 2) dx$ is :

- (A) $x^3 + x^2 + 2x + C$ (B) $x^6 + x^2 + 2x + C$ (C) $x^4 + x^3 + 2x + C$ (D) $x^3 + x^2 + x + C$

22. Find $\int_0^1 (5x^2 + 3x + 2) dx$

- (A) 20 (B) 30 (C) 40 (D) 10

23. In X-ray crystallography, the Bragg equation relates the distance d between successive layers in a crystal, the wavelength of the X-rays λ , an integer n and the angle through which the X-rays are scattered θ in the equation :

$$\lambda = \frac{2d}{n} \sin\theta$$

What is the rate of change of λ with θ ?

- (A) $\frac{2d}{n} \cos\theta$ (B) $\frac{2d}{n} \tan\theta$ (C) $\frac{2d}{n} \operatorname{cosec} \theta$ (D) none of these

24. For $y = a \ln(bx)$ find $\frac{dy}{dx}$

- (A) $\frac{b}{x}$ (B) $\frac{-b}{x}$ (C) $\frac{-a}{x}$ (D) $\frac{a}{x}$

25. Differentiate the y where $y = e^x + 4x^6$.

- (A) $e^x + 24x^6$ (B) $e^x + 24x^5$ (C) $e^x + 24x^4$ (D) $e^x + 6x^4$



26. Find the following integral $\int \frac{x^2 + 2x^3 - 4x^4}{x^3} dx$
- (A) $x + 2x - 2x^2 + C$ (B) $\ln|x| + 2x - 2x^2 + C$
 (C) $\ln|x| + x - 2x^2 + C$ (D) $\ln|x| + 2x - 2x + C$
27. Find integral of $\int e^{6x} dx$
- (A) $\frac{e^{6x}}{x} + c$ (B) $\frac{e^{6x}}{6} + c$ (C) $\frac{e^x}{x} + c$ (D) none of these
28. $\int \cos(4x) dx$
- (A) $\frac{\sin(4x)}{4} + c$ (B) $\frac{\sin(4x)}{x} + c$ (C) $\frac{\sin(x)}{4} + c$ (D) $\frac{\cos(4x)}{4} + c$
29. A curve of gradient 4×5 passes through the point (1, 2). What is the full equation of the line ?
- (A) $\frac{2}{3}x^6 + \frac{4}{2}$ (B) $\frac{2}{3}x^6 + \frac{2}{3}$ (C) $\frac{2}{3}x^6 + \frac{3}{4} C$ (D) $\frac{2}{3}x^6 + \frac{4}{3} C$
30. Find the dot product of $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} \sqrt{2} \\ \sqrt{2} \end{pmatrix}$
- (A) $\sqrt{3}$ (B) $\sqrt{2}$ (C) $\sqrt{5}$ (D) $\sqrt{8}$

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