FYUP-B.SC. (HONS.) CHEMISTRY PROGRAMME
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V SEMESTER EXAMINATION DECEMBER 2024
PAPER CODE: BCH DSC 503 TH
TITLE: QUANTUM CHEMISTRY & ELECTROCHEMISTRY

(Write your roll no. at the top immediately on receipt of this question paper)

Time: **2.5 Hours** Maximum Marks: **60**

Note: ***Attempt all the questions marks of each question given in parenthesis. All parts of a question must be attempted in continuation. Start answer of a fresh question on a new page. Cite examples and draw labelled diagrams wherever necessary.***

SECTION A

	BTL-	CLO	PLO
Attempt *All* of the following: **(15 x 1 = 15) Marks**			
1. The Debye-Huckel-Onsager treatment explains the conductance of electrolyte solutions and accounts for _____ interactions in solution.	1/2	1/2	1/2
2. The _____ equation is a fundamental equation in quantum mechanics, which can be applied to a free particle or a particle-in-a-box, leading to a _____ of energy levels.	1/2	1/2	1/2
3. What is degeneracy in quantum mechanics?	1/2	1/2	1/2
4. The _____ model assumes fixed bond lengths and describes the rotational motion of diatomic molecules, with energy levels determined by the _____ equation in spherical polar coordinates.	1/2	1/2	1/2
5. Show that the commutator $[x, \frac{\partial}{\partial x}] = -1$.	1/2	1/2	1/2
6. If $\hat{A}$ and $\hat{B}$] cap are two operators such that $[\hat{A}, \hat{B}] = 1$, show that $[\hat{A}, \hat{B}2] = 2\hat{B}$.	1/2	1/2	1/2
7. Show that $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$	1/2	1/2	1/2
8. Show that $[\hat{A}2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$	1/2	1/2	1/2
9. Explain Heisenberg uncertainty principle.	1/2	1/2	1/2
10. _____ represent the fraction of the total current carried by a specific ion in an electrolyte.	1/2	1/2	1/2
11. Overpotentials are extra potentials required to drive an electrochemical reaction, and are related to _____ losses in the system.	1/2	1/2	1/2
12. The exchange current density represents the current at equilibrium and is related to the rate of the _____ reaction.	1/2	1/2	1/2
13. The Lippmann equation relates surface excess charge to _____, and can be used to study the electrocapillarity of interfaces.	½	1/2	1/2
14. The Hodges-Huxley equations are used to model the electrical activity of _____ cells.	1/2	1/2	1/2
15. _____ are used to detect the endpoint of a titration by measuring the _____ between two electrodes.	1/2	1/2	1/2

SECTION B

Attempt **any two** of the following: **(2x10=20)** Marks			
1. Explain the Faradays laws of electrolysis and its applications? How do we measurement of conductivity for an electrolytic solution? A solution of $CuSO_4$ is electrolysed for 20 min with a current of 4.5 A. What is the mass of Cu deposited at the electrode?	5/6	5/6	5/6/7
2. How does the "Particle in a One-Dimensional Box" model illustrate the concept of quantized energy levels and their relationship to particle confinement within a limited space?	5/6	5/6	5/6/7

3. Find the expressions for the following operators:	5/6	5/6	5/6/7
A. $(\frac{\partial}{\partial x}+x)^2$ B. $(\frac{\partial}{\partial x}-x)^2$			
C. $(\frac{\partial}{\partial x}+x)((\frac{\partial}{\partial x}-x)$ D. $(\frac{\partial}{\partial x}-x)((\frac{\partial}{\partial x}+x)$			
4. Describe the thermodynamics of electrified interfaces and derive the Lippmann equation for electro-capillarity. How can surface excess be determined experimentally?	5/6	5/6	5/6/7

SECTION C

Attempt *all* questions **(5x5=25 Marks)**

III. Attempt the following: **(5x5=25)**	5/6	5/6	5/6/7
1. What is the Nernst equation and why is it important?			
OR			
Show that the commutator $[\widehat{Xn}], \widehat{px}]=\frac{ih}{2}$ n x^{n-1} where n is a positive integer.			
2. How much silver (Ag) is deposited when a current of 2.0 A is passed through a solution of silver nitrate ($AgNO_3$) for 30 minutes? (Given: Molar mass of Ag = 107.87 g/mol, n=1, Faraday constant F=96500 C/mol).	4/5/6	4/5/6	4/5/6
OR			
Discuss the various postulates of quantum mechanics?			
3. Derive the Butler-Volmer equation and explain its significance in electrochemical kinetics. How does the Tafel plot help in determining kinetic parameters?	5/6	4/5/6	5/6/7
OR			
Indicate which of the following functions are acceptable as wave functions:			
(i) $\psi = x$ (ii) $\psi = x^2$ (iii) $\psi = \sin x$			
(iv) $\psi = e^x$ (v) $\psi = e^{-x}$ (vi) $\psi = e^{-x^2}$ and			
(iv) $\psi = \tan x$			
4. What is the structure of electrified interfaces? Discuss the Guoy-Chapman, Stern, and other advanced models used to describe it.	3/4/5	3/4/5/6	3/4/5
OR			
Assuming that the ionic character in H-Br bond is 12%, calculate the fraction of the contribution of ionic character to the valence bond wave function.			
5. Explain the Debye-Huckel-Onsager theory for electrolyte solutions and its extension. How does it account for ion-solvent interactions?	3/4/5	3/4/5	3/4/5
OR			
What is the liquid junction potential, and how does it affect electrochemical measurements?			
