

COURSES OFFERED BY DEPARTMENT OF CHEMISTRY**B Sc. Physical Sciences**

**Undergraduate Programme of study
(with Chemistry as the Major Disciplines)**

Semester-wise Distribution of Discipline Specific Core (DSC) Courses

DISCIPLINE CORE COURSES –02 (4 Credits each)			
SEMESTER	COURSE CODE	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits
VII	DSC-19	Chemistry of d- and f- block elements, Advanced Organic Spectroscopy and Quantum Chemistry	T=3 P=1
VIII	DSC-20	Catalysis, Photocatalysis, Application of Reagents in Organic Synthesis and Statistical Thermodynamics	T=3 P=1

DISCIPLINE SPECIFIC ELECTIVE COURSES – (4 Credits each)			
SEMESTER	COURSE CODE	NAME OF THE COURSE	CREDITS T=Theory Credits P=Practical Credits
VII	Common Pool of DSE Courses applicable for both B.Sc. Physical Sciences and B.Sc. Life Sciences		
	DSE-14	Industrial Chemicals and Environment	T=2 P=2
	DSE-15	Advanced Stereochemistry	T=2 P=2
	DSE-16	Reactive Intermediates of Organic Chemistry	T=2 P=2
	DSE-17	Molecular Spectroscopy and Structural Analysis	T=2 P=2
	DSE Course applicable specifically for B.Sc. Physical Sciences		
	DSE-18 PS	Introductory Interfacial Electrochemistry	T=2 P=2
VIII	Common Pool of DSE Courses applicable for both B.Sc. Physical Sciences and B.Sc. Life Sciences		
	DSE-19	Fundamentals of Natural Products	T=2 P=2
	DSE-20	Fundamentals of Medicinal Chemistry	T=2 P=2
	DSE-21	Computational Chemistry	T=2 P=2
	DSE-22	Machine Learning and Artificial Intelligence in Chemistry*	T=2 P=2
	DSE Course applicable specifically for B.Sc. Physical Sciences		
	DSE-23 PS	Crystalline Solids: Properties and Methods of Analysis	T=2 P=2
	DSE-24 PS	Coordination Chemistry, Reaction Mechanism and Spectral properties	T=2 P=2

* For syllabus content of Discipline Specific Elective-22 (DSE-22) “Machine Learning and Artificial Intelligence in Chemistry” refer to DSE syllabus of B.Sc. (H) Chemistry.

Note: A student, studying in 4th year of B.Sc. Physical Science/Life Science Programme, desirous of opting any *Discipline Specific Elective* (DSE) Course from progression of DSE courses available in Semester III-VI of the programme, may be allowed to opt the same in the VIIth or VIIIth semester.

DISCIPLINE SPECIFIC CORE COURSE - 19 (DSC-19): Chemistry of d- and f-Block Elements, Advanced Organic Spectroscopy and Quantum Chemistry

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre- requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Chemistry of d- and f-block elements, Advanced Organic Spectroscopy and Quantum Chemistry (DSC-19)	04	03	-	01	Class 12th with Physics, Chemistry and Maths	--

Course Objectives

The objectives of this course are as follows:

- To provide thorough knowledge about the d- and f- block elements with respect to the general group trends, physical and chemical properties of these elements.
- To impart the knowledge about synthetic methods and principles of chromatography.
- Understanding spectroscopic techniques and their application in the structural elucidation of organic molecules.
- To explain the concept of linear Hermitian operators and commutation of operators and applications.
- To apply the postulates for deriving equations of various models and extend it to hydrogen atom and hydrogen like atoms.
- To explain the valence bond and molecular orbital theories and their applications to simple molecules

Learning outcomes

By studying this course, students will be able to:

- Analyse the important properties of transition metals, lanthanoids, and actinoids
- Understand Latimer diagrams to predict and identify species which are reducing, oxidizing and tend to disproportionate and calculate skip step potentials.

- Apply the principles of synthesis of Inorganic compounds and chromatographic separation of metal ions.
- Develop an understanding of the basic principles of NMR spectroscopy, such as chemical shift, coupling constant, and anisotropy, and describe how they are affected by molecular structure, and identify organic compounds by analysis and interpretation of spectral data.
- Develop an understanding of quantum mechanical operators, quantization, probability distribution, uncertainty principle
- Understand Schrodinger equations for different types of systems
- Analyse different wavefunctions and probability distribution curves.

UNIT- 1: Chemistry of Transition Elements

(15 Hours)

General group trends with special reference to electronic configuration, colour, variable valency, magnetic properties, catalytic properties, and ability to form complexes. Stability of various oxidation states and EMF (Latimer diagrams), Frost diagrams of Mn and Cr. A brief discussion of differences between the first, second and third transition series

A brief discussion of electronic configuration, oxidation states, colour, spectral and magnetic properties. Lanthanoid contraction (causes and effects), separation of lanthanoids by ion exchange method.

UNIT-2: Spectroscopic Techniques in Organic Chemistry

(15 Hours)

Recapitulation of the Spectroscopic Techniques (UV- VIS, IR, and ^1H NMR)

Carbon-NMR Spectroscopy

Resolution and multiplicity of ^{13}C NMR, ^1H -decoupling, noise decoupling, broadband decoupling; Deuterium, fluorine, and phosphorus coupling; NOE signal enhancement, Off resonance, proton decoupling, Structural applications of CMR. DEPT and general introduction about 2D NMR.

Mass Spectrometry

Theory, Fourier transform mass spectrometry instrumentation (FTMS); Unit mass and molecular ions; Important terms singly, doubly/multiple charged ions, metastable peak, base peak, isotopic mass peaks, relative intensity; Recognition of M^+ ion peak; Nitrogen rule; Rule of 13; Ionization methods (EI and ESI). General fragmentation rules: McLafferty rearrangement, ortho effect.

ESR Spectroscopy

Basic Principles and applications for organic Compounds.

Structure Elucidation

Structure elucidation of Organic Compounds Using UV, IR, NMR, and Mass Spectra.

Unit-3: Properties of operators, Particle in a Box, Harmonic Oscillator and Hydrogen Atom

(6 Hours)

Linear and Hermitian operators, Turn-over rule, Commutation of operators, and Uncertainty principle. Angular momentum operators, Eigenvalues and eigenfunctions, Particle in a box (3-D) and ring, and the concept of degeneracy.

Calculation of various average values ($\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$ and $\langle p^2 \rangle$) for simple harmonic oscillator. Calculation of the probabilities and most probable values of hydrogen 1s wavefunction.

Unit-4: Approximation Methods, Many Electrons Atom and Chemical Bonding (9 Hours)

First order time-independent perturbation theory for non-degenerate states, Variation theorem and variational methods. Use of these methods illustrated with some examples (particle in a box with a finite barrier, He atom).

Indistinguishability of the electrons and their intrinsic spin, spatial and spin wavefunctions, Pauli's Exclusion principle. Many-electron atom (Qualitative discussion).

Chemical bonding: Born-Oppenheimer approximation. Setting up of wavefunction of H_2^+ using Valence bond theory approach and qualitative discussion of solutions. Linear Combination of Atomic Orbitals (LCAO), salient features of MO theory and setting up of wavefunction of H_2 .

Practical:

Credits: 01

(Laboratory periods: 15 classes of 2 hours each)

PART A : INORGANIC CHEMISTRY

Inorganic Preparations

1. Potassium aluminium sulphate $KAl(SO_4)_2 \cdot 12H_2O$ (potash alum} or Potassium chromium sulphate $KCr(SO_4)_2 \cdot 12H_2O$ (chrome alum}.
2. Manganese phosphate and
3. Sodium peroxoborate

Paper chromatographic separation of following metal ions (minimum two should be done):

4. Ni(II) and Co(II)
5. Cu(II) and Cd(II)
6. Fe(III) and Al(III)

PART B: ORGANIC CHEMISTRY

(Note: Spectra to be provided wherever required)

7. Diels-Alder reaction between maleic anhydride and anthracene and identification of the product using IR and NMR Spectroscopy.
8. Knoevenagel condensation between aromatic aldehydes (benzaldehyde/*p*-nitro benzaldehyde) and active methylene compounds (malononitrile/ethyl cyanoacetate/diethylmalonate) and identification of the product using IR and NMR Spectroscopy.
9. Differentiate between maleic and fumaric acid solutions by UV spectroscopy.

10. Demonstration of the separation of the mixture of *p*-nitrophenol and *o*-nitrophenol by column chromatography and their characterization by melting point and spectroscopic techniques.

PART C: PHYSICAL CHEMISTRY

11. Plot the radial wavefunctions and probability distribution for H atom's 1s, 2s, 2p orbital using software i.e. MS-EXCEL.
12. (i) Draw probability plots for a particle in a 1-dimensional box for different values of quantum number *n* - commenting on the number of points of zero probability and then correlate them with the correspondence principle.
(ii) Calculate the bond length of conjugated dye molecules (i.e., cyanine/ β -carotene) using particle in 1D box model.
13. (i) Setting up of Schrödinger equation of Many-electron atoms and cite limitations to carry out exact solution of the problem.
(ii) Carry out calculation of various average values ($\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$ and $\langle p^2 \rangle$) for simple harmonic oscillator using MS-EXCEL.
14. Demonstrate the variational treatment of hydrogen molecule ion and also exhibit Valence bond and Molecular orbital (LCAO) treatment of hydrogen molecule. Calculation of HOMO and LUMO energies using computational software; Comparison of HOMO and LUMO energies relative to H-atom.
15. Demonstration of shapes and electronic features of bonding and antibonding σ and π orbitals on a visualization software.

Essential/recommended readings

Theory

1. Lee, J. D. (2010), Concise Inorganic Chemistry, Wiley India.
2. Huheey, J.E.; Keiter, E.A.; Keiter, R. L.; Medhi, O. K.(2009), Inorganic Chemistry- Principles of Structure and Reactivity, Pearson Education.
3. Atkins, P.W.; Overton, T.L.; Rourke, J.P.; Weller, M.T.; Armstrong, F.A. (2010), Shriver and Atkins Inorganic Chemistry, 5th Edition, Oxford University Press.
4. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), Inorganic Chemistry, 5th Edition, Pearson.
5. Pfennig, B. W. (2015), Principles of Inorganic Chemistry. John Wiley & Sons.
6. Cotton, F.A.; Wilkinson, G. (1999), Advanced Inorganic Chemistry, Wiley-VCH.
7. Das, A. K.; Das, M. (2014), Fundamental Concepts of Inorganic Chemistry, 1st Edition, Volume 1-3, CBS Publishers & Distributors Pvt. Ltd.
8. S. K. Ghuman, A.Sakthivel, D. T. Masram, M.Sathiyendiran, (2017) Electronic and Magnetic properties of transition and inner transition elements and their complexes,

Nova Science Publishers, New York.

9. Chandrashekhara, V. (2005), Inorganic and Organometallic Polymers, 5th Edition, Springer Publications.
10. Kemp, W. Organic Spectroscopy 3rd Ed., W. H. Freeman & Co. (1991).
11. Silverstein, R. M., Bassler, G. C. & Morrill, T. C. Spectroscopic Identification of Organic Compounds. John Wiley & Sons (1981).
12. Pavia, D. L.; Lampmann, G. M.; Kriz, G. S.; Vyvyan, J. R. Introduction to Spectroscopy. Cengage Learning (2014).
13. Organic Structures from spectra; L. D. Field, S. Sternhell and J R Kalman, John Wiley & Sons Ltd., 2007
14. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
15. Bakhshi, A. K. & Thakral P., Quantum Chemistry Simplified Vidyavani Foundation: New Delhi (2025) (ISBN: 9788196225107).
16. House, J.E. (2004), Fundamentals of Quantum Chemistry, 2nd Edition, Elsevier.
17. McQuarrie, D.A. (2016), Quantum Chemistry, Viva Books.
18. Atkins, P.W.; Paula, J.de. (2014), Atkin's Physical Chemistry Ed., 10th Edition, Oxford University Press.
19. Atkins, P.W.; Friedman, R. (2010), Molecular Quantum Mechanics, 5th Edition, Oxford University Press.

Practical:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. (1989), Vogel's Textbook of Quantitative Chemical Analysis, John Wiley and Sons,
2. Harris, D. C.; Lucy, C. A. (2016), Quantitative Chemical Analysis, 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. (2012), Quantitative Analysis, Sixth Edition, PHI Learning Private Limited.
4. Marr, G.; Rockett, B.W. (1972), Practical Inorganic Chemistry, Van Nostrand Reinhold.
5. Vogel, A. I. (2012). Quantitative Organic Analysis, Part 3, Pearson Education.
6. Mann, F. G., Saunders, B.C. (2009), Practical Organic Chemistry, Pearson Education.
7. Furniss, B. S., Hannaford, A.J., Smith, P.W.G., Tatchell, A. R. (2012), Vogel's Textbook of Practical Organic Chemistry, Fifth Edition, Pearson.
8. Ahluwalia, V.K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
9. Morrill, L. A., Kammeyer, J. K., & Garg, N. K. (2017). Spectroscopy 101: A practical introduction to spectroscopy and analysis for undergraduate organic chemistry laboratories. *J. Chem. Educ.* 94 (10), 1584-1586.
10. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, McGraw Hill Education, Vol 4, 5th Edition, McGraw Hill Education.
11. McQuarrie, D. A. (2008) Mathematics for Physical Chemistry University Science Books.
12. Mortimer, R. (2005) Mathematics for Physical Chemistry. 3rd Ed. Elsevier.
13. Steiner, E. (1996) The Chemical Maths Book Oxford University Press.

14. Yates, P. (2007) Chemical Calculations. 2nd Ed. CRC Press.
15. Levie, R. de, How to use Excel in analytical chemistry and in general scientific data analysis, Cambridge Univ. Press (2001) 487 pages.
16. Noggle, J. H. Physical Chemistry on a Microcomputer. Little Brown & Co. (1985).

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

DISCIPLINE SPECIFIC CORE COURSE - 20 (DSC-20): Catalysis, Photocatalysis, Application of Reagents in Organic Synthesis and Statistical Thermodynamics

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Catalysis, Photocatalysis, Application of Reagents in Organic Synthesis and Statistical Thermodynamics (DSC-20)	04	03	--	01	Class 12 th with Physics, Chemistry, Maths	--

Course Objectives

The objectives of this course are as follows:

- To impart basic knowledge of Organometallic compounds and catalysis,
- To enrich students with the knowledge of various types of bonding and structure of organometallic compounds and biocatalysts.
- To impart the theoretical and practical knowledge of catalysts with the view of their industrial applications.
- To facilitate chemical transformations by providing the necessary conditions and catalysis.
- To provide a brief foundational understanding of the core principles of statistical thermodynamics.
- To study the connection between macroscopic thermodynamics and microscopic quantum mechanics utilizing various statistical ensembles.
- To study Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac statistics with a brief, qualitative understanding and focus on their applications.
- To enable students to apply statistical concepts in key areas such as the standard model, chemical kinetics, and chemical equilibrium.

Learning outcomes

By studying this course, the students will be able to:

- Develop understanding on the role of catalyst in industrial applications.

- Gain sound knowledge of various types of catalyst.
- Develop skilled in the scientific method of planning, developing, conducting, reviewing and reporting experiments.
- Develop skilled concepts of industrial catalysis which will help them to explore new innovative areas of research
- Understand various reducing agents, oxidizing agents, and their applications in organic synthesis.
- Understand the conversion of specific functional groups without affecting others and maximize yields and selectivity for the desired products
- Understand the fundamental principles of statistical mechanics, including how they link microscopic behaviour to macroscopic properties of systems.
- Apply the Boltzmann distribution, Bose-Einstein statistics, and Fermi-Dirac statistics in various physical and chemical systems.
- Analyse and solve problems related to the thermodynamic properties of systems using partition functions.
- Explore the application of statistical mechanics to key areas such as chemical kinetics, chemical equilibrium, and random walk models in macromolecular systems.

UNIT- 1: Catalysis and Photocatalysis

(15 Hours)

General principles of catalysis, properties of catalysts, Mode of action of catalyst, Types of catalyst (homogeneous and heterogeneous catalysis), Deactivation and regeneration of catalysts, catalytic poison, Promoter, Turnover frequency, Turnover number, Specificity and selectivity.

Catalysis in environmental remediation, eco-friendly energy solutions and production of valuable chemicals.

Study of the following industrial processes, catalytic cycle and their mechanism:

1. Alkene hydrogenation (Wilkinson's Catalyst).
2. Synthetic gasoline (Fischer Tropsch reaction).
3. Polymerisation of ethene using Ziegler-Natta catalyst.
4. Wacker-Smith synthesis of aldehyde.

Photocatalysis: Basic principle, Mechanism, Types of Photocatalysts, band gap, tuning of band gap, doping, UV- visible light lamp source, UV-visible light filters, Water Splitting, Photoreduction and oxidation of water, Brief discussion of example of Photocatalysis: Photosynthesis, Pollutant degradation, Hydrogen production, CO₂ conversion.

UNIT- 2: Synthesis and applications of Reagents in Organic Synthesis

(15 Hours)

Synthesis and applications of BuLi, Grignard, organoaluminium, and organozinc reagents.

Triacetoxyborohydride, Lead Acetate, Phenyl iodine (III) diacetate (PIDA), DCC, Tamao-Fleming Oxidation; Dimethyldioxirane (DMDO) Oxidation; DMSO (Barton modification & Swern Oxidation); Oxidation of organic compounds using thallium nitrate, selenium dioxide, phase transfer catalyst, crown ethers, KMnO₄, PCC, OsO₄, CrO₃, K₂Cr₂O₇.

Applications of hydroboration (reductions, oxidations, and carbonylation): Diborane, 9-BBN.

UNIT- 3: Elements of Statistical Mechanics (10 Hours)

Microstates, Configurations, tossing of coins, rolling of dices and spin of electrons in absence of magnetic field, most probable thermodynamic probability, Stirling's Approximation, Concepts of ensembles, Microcanonical, Canonical ensembles, Qualitative Discussion of translational, vibrational, and rotational Partition functions, Maxwell-Boltzmann, Bose-Einstein, and Fermi-Dirac Statistics (Qualitative discussions)

UNIT- 4: Conventional Transition State Theory and Brownian Motion (5 Hours)

Conventional transition state theory in terms of molecular partition functions, gas phase equilibrium constant in terms of partition function, 1-D random walk model, Brownian Dynamics (Qualitative discussion only).

Practicals:**Credits: 01****(Laboratory periods:15 classes of 2 hours each)****PART A : INORGANIC CHEMISTRY**

1. Synthesis of "Zeolite A" catalyst.
2. Zeolite Hydrogen-Y or dil.HCl/dil.H₂SO₄ as a Catalyst for the Preparation of an Ester.
3. Catalytic Synthesis of biaryl.
4. Catalytic Transfer Hydrogenation of Castor Oil
5. Reduction of Nitrobenzene
6. Synthesis of Cu₂O, TiO₂, Fe₃O₄, ZnO, and NiO Nanoparticles and characterization by UV/Vis spectroscopy.
7. Photocatalytic degradation of Methylene Blue dye using Cu₂O, TiO₂, Fe₃O₄, ZnO, and NiO Nanoparticles and UV/Vis studies.

PART B : ORGANIC CHEMISTRY

8. Identification of the product based on Melting point and spectroscopic techniques (IR, ¹HNMR, and ¹³C NMR spectroscopy, data to be provided).
9. Synthesis of 1,2,3,4-tetrahydrocarbazole from cyclohexanone.
10. Reduction of *p*-nitrobenzaldehyde using NaBH₄
11. Synthesis of 2,3-diphenylquinoxaline from benzil and *ortho*-phenylenediamine.
12. Oxidation of benzyl alcohol by KMnO₄.

PART C: PHYSICAL CHEMISTRY

13. Study of kinetics of the iodination of acetone in the presence of acid by the *Initial Rate Method*.
14. Statistical Treatment of Error Analysis (Null Hypothesis, T-test, F-test, Q-test (criteria for rejection of hypothesis) Statistical analysis of laboratory data.

15. Determination of standard deviation, mean, and maximum absolute errors, root-mean-square deviation (error), and Correlation coefficient of linear straight-line plot.

Essential/recommended readings

Theory:

1. Huheey, J. E.; Keiter, E.A.; Keiter; R. L.; Medhi, O.K. (2009), Inorganic Chemistry- Principles of Structure and Reactivity, Pearson Education.
2. Cotton, F.A.; Wilkinson, G. (1999), Advanced Inorganic Chemistry, Wiley-VCR.
3. Jens Hagen (2015) Industrial Catalysis: A Practical Approach Wiley-VCR Verlag GmbH&Co
4. Carruthers, W. Modern Methods of Organic Synthesis. Cambridge University Press (1996).
5. Carey, F.A. & Sundberg, R. J. Advanced Organic Chemistry, Parts A & B, Plenum: U.S. (2004).
6. Jonathan Clayden, Nick Greeves, Stuart Warren. Organic Chemistry. Oxford. (2000)
7. McQuarrie, D. A. *Statistical Mechanics*, Viva Books Pvt. Ltd.: New Delhi (2003).
8. Reif, Frederick., Fundamentals of Statistical and Thermal Physics, McGraw-Hill, (1965).
9. Huang, Kerson, Statistical Mechanics, 2nd ed., Wiley (1987).
10. Pathria, R. K., and Paul D. Beale, Statistical Mechanics, 3rd ed., Elsevier (2011).
11. Pal, Palash B., (2008) Statistical Mechanics: Principles and Applications, Narosa Publishing House.
12. Bagchi B., (2018) Statistical Mechanics for Chemistry and Material Science, CRC Press.
13. L. D. Landau and E. M. Lifshitz, (2005) Statistical Mechanics, Part I, Butterworth-Heinemann, 3rd ed.
14. Laidler, K. J. (1997) *Chemical Kinetics* 3rd Ed., Benjamin Cummings.
15. Atkins, P. W. & Paula, J. de (2006) *Atkin's Physical Chemistry* 8th Ed., Oxford University Press.
16. McQuarrie, D. A. & Simon, J. D. (2001) *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books.

Practical:

1. Williams, D. J.; Huck, B. E.; Wilkinson, A. P. First-Year Undergraduate Laboratory Experiments with Zeolites Chem. Educator 2002, 7, 33-36.
2. Coker, E. N.; Davis, P. J.; Experiments with Zeolites at the Secondary-School Level: Experience from The Netherlands Journal of Chemical Education 1999, 76, 10, 1417.
3. Hanson RW. Catalytic transfer hydrogenation reactions for undergraduate practical programs. J Chem Educ. 2009, 74, 430.
4. Alwaseem H, Donahue CJ, Marincean S. Catalytic transfer hydrogenation of castor oil. J Chem Educ. 2014; 91, 575-8.
5. Ramesh R; Rajendran A.; Photocatalytic dye degradation activities of green synthesis of cuprous oxide nanoparticles from Sargassum wightii extract, Chemical Physic Impact, 2023, 6, 100208.

6. Ahluwalia, V. K., Dhingra, S. (2004), Comprehensive Practical Organic Chemistry: Qualitative Analysis, University Press.
7. Ahluwalia, V. K., Aggarwal, R. (2004), Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press
8. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–I, I K International Publishing house Pvt. Ltd, New Delhi
9. Pasricha, S., Chaudhary, A. (2021), Practical Organic Chemistry: Volume–II, I K International Publishing house Pvt. Ltd, New Delhi
10. Khosla, B.D.; Garg, V.C.; Gulati, A. (2015), Senior Practical Physical Chemistry, R. Chand & Co, New Delhi.
11. McQuarrie, D. A. & Simon, J. D. (2001) *Physical Chemistry: A Molecular Approach* 3rd Ed., Univ. Science Books.

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SEMESTER VII

**Discipline Specific Elective Courses (Common Pool) applicable for both
B.Sc. Life Sciences and B.Sc. Physical Sciences**

**Discipline Specific Elective Course – 14 (DSE-14):
Industrial Chemicals and Environment****

****For syllabus content of Discipline Specific Elective-14: (DSE-14) “Industrial Chemicals and Environment” refer to the syllabus content of DSE-14 of B Sc. Life Sciences Programme.**

Discipline Specific Elective Course – 15 (DSE-15):
Advanced Stereochemistry**

****For syllabus content of Discipline Specific Elective-15: (DSE-15) “Advanced Stereochemistry” refer to the syllabus content of DSE-15 of B Sc. Life Sciences Programme.**

**Discipline Specific Elective Course – 16 (DSE-16):
Reactive Intermediates of Organic Chemistry****

****For syllabus content of Discipline Specific Elective-16: (DSE-16) “Reactive Intermediates of Organic Chemistry” refer to the syllabus content of DSE-16 of B Sc. Life Sciences Programme.**

**Discipline Specific Elective Course – 17 (DSE-17):
Molecular Spectroscopy and Structural Analysis****

****For syllabus content of Discipline Specific Elective-17: (DSE-17) “Molecular Spectroscopy and Structural Analysis” refer to the syllabus content of DSE-17 of B Sc. Life Sciences Programme.**

**Discipline Specific Elective Courses Applicable Specifically for
B.Sc. Physical Sciences**

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE

**Discipline Specific Elective Courses –18 PS (DSE-18 PS):
Introductory Interfacial Electrochemistry**

COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Introductory Interfacial Electrochemistry (DSE-18 PS)	04	02	--	02	Class 12 th with Physics, Chemistry, Mathematics	--

Course Objectives

The objectives of this course are as follows:

- To discuss the electrochemical cells and Faradaic and Nonfaradaic Processes.
- To develop an understanding of electrical double layer and various equivalent circuit models of electrical double layer.
- To enable learners to have an insight into electrode kinetics and evaluation of kinetic parameters.
- To explain nature of electrode processes using cyclic voltammograms.
- To provide hands-on experience with setting up of electrochemical cells, quantitative estimation and evaluation of important physical quantities.

Learning outcomes

By studying this course, the students will be able to:

- Develop an understanding of working, counter electrode and differentiate between various reference electrodes along with the nature of electrode process.
- Understand the concept of electrical double layer and various equivalent models of the electrical double layer.

- Understand kinetics parameters from Tafel plot and thus demonstrate understanding of electrode kinetics, Butler-Volmer equation; its physical implications and cyclic voltammograms.
- Understand various applications of electrochemistry i.e. electrocatalysis, transport in electrolyte solution, conversion and storage of electrochemical energy.
- Perform hands-on laboratory exercise and interpret results of important electrochemical techniques i.e. cyclic voltammetry.

Theory:

Unit 1 Electrochemical Cells and Reaction - (6 Hours)

Working and Counter Electrodes, Reference Electrodes: standard hydrogen electrode (SHE), or normal hydrogen electrode (NHE), saturated calomel electrode (SCE), silver-silver chloride electrode, potential of zero charge, open-circuit potential of the cell, overpotentials. Faradaic and Nonfaradaic Processes: ideal polarized (or ideal polarizable) electrode, Capacitance and Charge of an Electrode, supporting electrolyte.

Unit 2: Electrical Double Layer (8 Hours)

Description of the Electrical Double Layer: inner and outer compact layer Helmholtz, or Stern layer, Diffuse Layer, specifically and non-specifically adsorbed ions, Potential profile across the double-layer region in the absence of specific adsorption of ions, Equivalent circuit models of EDL, Gouy-Chapman Model, qualitative Graham-Devanathan-Mottwatts, Tobin, Bockris, Devanathan model.

Unit 3: Electrode Kinetics (8 Hours)

Electrode Kinetics: Formal and Equilibrium Potentials, Overpotentials, Derivation of Butler-Volmer equation and its physical implications, Exchange current density and transfer coefficient, Evaluation of kinetics parameters from Tafel plot. Explain reversible, quasireversible, irreversible and capacitive response using cyclic voltammograms.

Unit 4: Applications of Electrochemistry (8 Hours)

Electrocatalysis: Influence of various parameters on water splitting, HER and OER.

Corrosion: Introduction to corrosion, forms of corrosion, General description of Corrosion monitoring and prevention.

Transport in Electrolyte Solution: Qualitative discussion of Fick laws and equations of Einstein on diffusion.

Conversion and Storage of Electrochemical Energy: Fuel cells, Supercapacitors and Li ion batteries, Redox flow batteries.

Practicals:

Credits: 02

(Laboratory periods:15 classes of 4 hours each)

1. Conductometric Titration of a Charge Transfer System, the formation of charge transfer complex between an electron donor and acceptor is studied and the stoichiometry of the complex is determined by following the variation of conductance of the solution with concentration of the donor and acceptor.
2. Effect of ionic strength on reaction rate (persulfate-iodine reaction).

3. Potentiometric determination of solubility and solubility product of AgCl(s) in water.
4. Potentiometric determination of mean ionic activity coefficient of HCl at different concentrations.
5. Potentiometric titration of Phosphoric acid vs NaOH .
6. Determination of dissociation constant of acetic acid from its potentiometric titration curve.

Hands-on/Demonstration/ Instruction Mode*: Demonstration/ Discussion of working principle/ Hands-on with substantial literature analysis/ Laboratory exercise.

7. Record cyclic voltammogram for the electrochemical capacitors (electric double layer) response with varying scan rates,
 - i) plot anodic and cathodic plateau currents vs scan rates.
(Use aqueous solution of 1.5 M NaNO_3)
8. Record cyclic voltammogram for a reversible heterogeneous electron transfer system with varying scan rates,
 - (i) Determine anodic and cathodic peak current ratio.
 - (ii) Determine anodic and cathodic peak potential difference.
 - (iii) Plot peak current vs square root of scan rates.
(Use aqueous solution of 10 mM $\text{K}_4\text{Fe}(\text{CN})_6 + \text{K}_3\text{Fe}(\text{CN})_6 + 1.5 \text{ M NaNO}_3$)
9. Record cyclic voltammogram for a quasi-reversible heterogeneous electron transfer system with varying scan rates,
 - (i) Determine anodic and cathodic peak current ratio.
 - (ii) Determine anodic and cathodic peak potential difference.
 - (iii) Plot peak current vs square root of scan rates.
(Use aqueous solution of 10 mM $\text{Fe}(\text{NH}_4)_2 (\text{SO}_4)_2 + \text{Fe}(\text{NH}_4)(\text{SO}_4)_2 + 1 \text{ M HClO}_4$)
10. Record the CV of aqueous solution of sulphuric acid (0.5 M) at Pt electrode as working electrode and counter electrode.
 - (i) Interpret and explain various peaks and region of the CV and their significance.
Determine the area and roughness factor of the electrode by Pt oxide region.

*[pre-recorded data for computer simulation may also be shared for visualization analysis and interpretation on MS-Excel]

Laboratory Activities

11. Assembling a simple electrochromic device from household materials and visualization of the colour change of curcumin.
(<https://pubs.acs.org/doi/10.1021/acs.jchemed.2c00176>.)
12. Design concentration cells to demonstrate whether
 - (i) Iron under the water surface has the same Corrosion Level at any part?
 - (ii) Copper Sheets be Galvanized with Zinc without an External Power Supply?
(<https://pubs.acs.org/doi/10.1021/acs.jchemed.0c01408>.)

Essential/recommended readings

Theory:

1. Bard, A. J. Faulkner, L. R. Electrochemical Methods: Fundamentals and Applications, 2nd Ed., John Wiley & Sons: New York, 2002.

2. Oldham, K. B., Myland, J. C. and Bond, A. M. *Electrochemical Science and Technology: Fundamental and Applications*, John Wiley & Sons, Ltd. (2012).
3. Bockris, J. O' M. & Reddy, A. K. N. *Modern Electrochemistry 1: Ionics* 2nd Ed., Springer (1998).
4. Bockris, J. O' M. & Reddy, A. K. N. *Modern Electrochemistry 2B: Electrodics in Chemistry, Engineering, Biology and Environmental Science* 2nd Ed., Springer (2001).
5. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. *Modern Electrochemistry 2A: Fundamentals of Electrodics* 2nd Ed., Springer (2001).
6. Brett, C. M. A. & Brett, A. M. O. *Electrochemistry*, Oxford University Press (1993).
7. Koryta, J., Dvorak, J. & Kavan, L. *Principles of Electrochemistry* John Wiley & Sons: NY (1993).
8. Bagotsky, V.S., *Fundamentals of electrochemistry* 2nd Ed. Wiley – Interscience, (2006)
9. Hamann, Carl H., Hamneff, Andrew & Vielstich, Wolf., *Electrochemistry*, 2nd Ed. (2007)

Practical:

1. B. D. Khosla, V. C. Garg, A. Gulati, *Senior Practical Physical Chemistry*, R. Chand & Co, New Delhi.
2. Holze R., (2019) *Experimental Electrochemistry: A laboratory Textbook*, Wiley-VCH.
3. Elgrishi, N.; Rountree, K. J.; McCarthy, B. D.; Rountree, E. S.; Eisenhart, T. T.; Dempsey, J. L. A Practical Beginner's Guide to Cyclic Voltammetry, *J. Chem. Educ.* **2018**, 95, 2, 197–206.
4. Field, R. J.; Schneider, F. W. Oscillating Chemical Reactions and Nonlinear Dynamics, *J. Chem. Educ.* **1989**, 66, 3, 195–204.
5. Rozman M, Alif M, Bren U., Lukšič M., Electrochromic Device Demonstrator from Household Materials, *J. Chem. Educ.* 99, 10, 3595-3600.
6. Ling Y., Chen P., **2022**, Wang J., Chen K, Ren H. Design, Implementation, and Evaluation of a Scientific Modeling Course on Concentration Cells, *J. Chem. Educ.* **2021**, 98, 4, 1163-1173

Note: Minimum 6 hands-on exercise to be performed.

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

SEMESTER VIII

**Discipline Specific Elective Courses (Common Pool) applicable for both
B.Sc. Life Sciences and B.Sc. Physical Sciences**

**Discipline Specific Elective Course – 19 (DSE-19)
Fundamentals of Natural Products****

****For syllabus content of Discipline Specific Elective-19: (DSE-19) “Fundamentals of Natural Products” refer to the syllabus content of DSE-19 of B Sc. Life Sciences Programme.**

DISCIPLINE SPECIFIC ELECTIVE COURSE – 20 (DSE-20)
Fundamentals of Medicinal Chemistry**

****For syllabus content of Discipline Specific Elective-20: (DSE-20) “Fundamentals of Medicinal Chemistry” refer to the syllabus content of DSE-20 of B Sc. Life Sciences Programme.**

DISCIPLINE SPECIFIC ELECTIVE COURSE - 21 (DSE-21)
Computational Chemistry**

****For syllabus content of Discipline Specific Elective-21: (DSE-21) “Computational Chemistry” refer to the syllabus content of DSE-21 of B Sc. Life Sciences Programme.**

**DISCIPLINE SPECIFIC ELECTIVE COURSE - 22 (DSE-22):
Machine Learning and Artificial Intelligence in Chemistry***

***For syllabus content of Discipline Specific Elective-22: (DSE-22)** “Machine Learning and Artificial Intelligence in Chemistry refer to the pool of DSE courses in 4th year syllabus of **B.Sc. (H) Chemistry**.

**DISCIPLINE SPECIFIC COURSES Applicable Specifically for
B.Sc. Physical Sciences**

**DISCIPLINE SPECIFIC ELECTIVE COURSE – 23 PS (DSE-23 PS):
Crystalline solids: Properties and Methods of Analysis**

**CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE
COURSE**

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Crystalline Solids: Properties and Methods of Analysis (DSE-23 PS)	04	02	--	02	Class 12th with Physics, Chemistry, Mathematics	--

Course Objectives

The objectives of this course are as follows:

- To analyse different crystal systems and understand their properties.
- To study Curie's and Curie-Weiss law and its application to paramagnetic and ferromagnetic materials, respectively.
- To understand the principles and application of basic instrumentation techniques.

Learning outcomes

By studying this course, the students will be able to:

- Distinguish between lattice, unit cell, and the 14 Bravais lattices, and understand their symmetry and properties.
- Interpret XRD patterns of NaCl, CsCl, and KCl to deduce structural information.
- Understand the Curie-Weiss law and its application to ferromagnetic materials.
- Analyse and interpretation of experimental data obtained through experimental techniques.

Theory:

Unit 1: Crystalline Solids

(9 Hours)

Classification and characteristics of crystalline solids, seven crystal systems. Fundamentals of lattice, unit cell and fourteen Bravais lattices. Types of closed-packed structures. Elementary idea of symmetry. Crystal's direction and planes, Miller indices.

Unit 2: Diffraction Methods

(9 Hours)

Bragg's law and Bragg's conditions. X-ray diffraction pattern of simple cubic systems i.e. NaCl, CsCl, and KCl, Laue method, Crystallite size (Scherrer equation) and Williamson-Hall method to determine lattice strains from diffraction patterns. Elementary idea of Thermogravimetric analysis (TGA).

Unit 3: Electronic Properties and Band Theory of Solids (6 Hours)

Introduction- metals, insulators, and semiconductors. Electronic structure, k-space and Brillouin zone, band structure of metals, insulators, and semiconductors.

Unit 4: Magnetic Properties (6 Hours)

Magnetic moment, Curie law, Curie-Weiss law, magnetic ordering, exchange Interaction, Hysteresis, anisotropy, paramagnetism, ferromagnetism, ferrimagnetism, antiferromagnetism

Practicals:

Credits: 02

(Laboratory periods:15 classes of 4 hours each)

1. Preparation of semiconducting TiO_2 / ZnO / CdSe / ZnSe / In_2S_3 and metal nanomaterials (Ag/ Cu/ Ni etc.) by any soft chemical approach (emulsion based, co-precipitation etc.). (Minimum two preparations)
2. Analysis of diffraction pattern obtained from Powder X-ray diffractometer. Identifying crystal phase, diffraction peaks with lattice planes for a given compound*.
3. Determination of approximate crystallite size using the given PXRD pattern of a known compound i.e. TiO_2 , ZnO etc by employing Scherrer equation*.
4. Determination of lattice strain using Williamson-Hall equation and from the measured PXRD pattern of a known inorganic compound for example, TiO_2 , ZnO etc.*
5. Determination of band gap of a semiconducting nanoparticle (in solution) using UV-visible spectrophotometer.
6. Thermogravimetric analysis of a known compound*. (Analysis of the thermal decomposition pattern of a hydrated salt like calcium sulfate pentahydrate, magnesium sulfate heptahydrate, etc.)
7. Determination of congruent composition and temperature of a binary system (e.g. diphenylamine-benzophenone/ Urea-resorcinol system).
8. Analysis of p-XRD data of a given set of Metals/ compounds* (Ag/Au/Cu/NaCl/CsCl) and confirmation of the type of the cubic system corresponding to given species.
9. Demonstrate the Principles, experimental setup, and instrumentation of TGA, and Interpretation of the analytical information from TGA curves*.

*[Diffraction patterns of known sample along with Standard JCPDS file (JCPDS: Joint Committee for Powder Diffraction Studies) be provided to students for analysis]

Essential/recommended readings

Theory:

1. Kapoor, K.L. (2015), A Textbook of Physical Chemistry, Vol 1, 5th Edition, Mc Graw Hill Education.
2. Levine I.N. (2009), Physical Chemistry 6th Edition, Mc Graw Hill Education.
3. Pillai S.O., (2022) Solid State Physics 6th Edition, New Age International Publishers.
4. Chakrabarty, (2022) D. K., Solid State Chemistry, 2nd Edition, New Age International Publishers.
5. West, A.R., (2022), Solid State Chemistry and its Applications, 2nd Edition, Wiley Inc.
6. Callister W. D., (2018) Materials Science and Engineering: An Introduction, 10th Edition, Willey Inc.
7. Keer H. V., (Reprint 2005), Principles of the Solid State, New Age International Publishers.

Practical:

1. Cullity, B. D. (2001) *Elements of X-ray Diffraction*, 3rd ed.; Prentice Hall.
2. Hammond, C. (2015) *The Basics of Crystallography and Diffraction*, 4th ed.; Oxford University Press.
3. Snyder, R. L. (1996) Jenkins, R. *Introduction to X-ray Diffractometry*; Wiley: New York.
4. Evans J. S. O., Evans I.R., Structure Analysis from Powder Diffraction Data: Rietveld Refinement in Excel, *J. Chem. Educ.* **2021**, 98, 2, 495-505.
5. Hulien M.L., Lekse J.W., Rosmus K. A., Devlin K. P., Glenn J.R., Wisneski S. D., Wildfong P., Lake C. H., MacNeil J. H. Aitken J. A., An Inquiry-Based Project Focused on the X-ray Powder Diffraction Analysis of Common Household Solids, *J. Chem. Educ.* **2015**, 92, 12, 2152-2156.
6. Bentley A. K., Farhoud M, Ellis A. B., Lisensky G.C., Nickel A-Marie L, Crone W. C., Template Synthesis and Magnetic Manipulation of Nickel Nanowires, *J. Chem. Educ.* **2005**, 82, 5, 765-768.
7. Oliveira M. L., Pagung E., Lorenzini L., Neves T.R., Pereira J.R.P., Ferreira S. A. D., Freitas M. B. J.G. de, Moura P. R.G., Lelis M. F. F., Synthesis of Iron Oxide Nanoparticles and their Application in Photo-Fenton Process: An Undergraduate Experiment in Chemistry, *J. Chem. Educ.* **2025**, 102, 1590-1597.
8. How to Characterize 4–90nm Size Gold Nanospheres with Experimental and Simulated UV–Vis and a Single SEM Image, *J. Chem. Educ.* **2023**, 100, 1589-1596.
9. <https://www.icdd.com/> (International Centre for Diffraction Data).

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.-

DISCIPLINE SPECIFIC ELECTIVE COURSE – 24 PS (DSE-24 PS)
Coordination Chemistry, Reaction Mechanism and Spectral properties

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Coordination Chemistry, Reaction Mechanism and Spectral properties (DSE-24 PS)	04	02	--	02	Class 12 th with Physics, Chemistry, Mathematics	--

Course Objectives

The Learning Objectives of this course are as follows:

- Solve problems from the basic and advanced concepts of transition metal chemistry
- Apply different bonding theories to explain the interaction between transition metals and ligands and predict the shape, stability, and optical and magnetic properties of complexes
- Design the most possible products and choose appropriate reaction condition to obtain the desired products in coordination compounds
- Appraise some natural phenomenon where reactions of coordination compounds are happening inside the human body and in plants enabling them to improve individual and societal health as well as environment.

Learning Outcomes

By the end of this course, students will be able to:

- Understand the advance theories to explain bonding in complexes.
- Attain knowledge of reaction mechanism of complexes.
- Understand the spectroscopic techniques to study structure and bonding in complexes.
- Develop skills in the scientific method of planning, developing, conducting, reviewing and reporting experiments.
- Understand concepts of industrial catalysis which will help them to explore new innovative areas of research.

Theory:

Unit 1: Ligand Field/ Molecular Orbital Theory (MOT) of Coordination Compounds

(10 Hours)

Limitations of CFT, Crystal field to ligand field, σ and π bonding and energy diagrams of octahedral, tetrahedral, square planar complexes, effect of ligand group orbitals on Δ , effect of charge of metal on Δ , spectrochemical series comparison from different theories.

Unit 2: Reaction Mechanism

(10 Hours)

Reaction mechanisms of metal complexes, Nucleophilic substitution reactions in octahedral complexes and their mechanisms, hydrolysis reactions, water exchange reactions, trans effect and its application, electron transfer reactions, inner sphere and outer sphere mechanisms, mixed valence complexes, redox reactions of metal complexes in excited states, role of spin-orbit coupling, life-times of excited states in these complexes.

Unit 3: Electronic Transitions and Selection Rules

(5 Hours)

Spin and Laporte selection rules of transitions, charge transfer transitions, LMCT and MLCT transitions, Intervalence charge transfer and inter ligand π - π^* charge transfer.

Unit 4: Spectral Properties

(5 Hours)

Nephelauxetic series, Orgel and Tanabe-Sugano diagrams, spin cross over, Jahn-Teller Distortions and Spectra,

Practicals:

Credits: 02

(Laboratory periods:15 classes of 4 hours each)

1. Estimation of Ca^{2+} in solution by (substitution method) using Erio-chrome black-T as indicator.
2. Estimation of Ca^{2+} / Mg^{2+} in drugs/ Milk/ Biological samples by Back titration.
3. Complexometric estimation of Zn^{2+} using Xylenol orange as indicator.
4. Complexometric estimation of Al^{3+} using Erio-chrome black-T as indicator.
5. Complexometric estimation of mixture of Zn^{2+} and Mg^{2+} in a sample solution using Xylenol orange and Eriochrome black-T as indicator
6. Complexometric estimation of mixture of Al^{3+} and Mg^{2+} in a sample solution using masking agent.
7. Estimation of BaSO_4 by EDTA back titration using Eriochrome black-T as indicator.
8. Measurement of 10 Dq by spectrophotometric method.
9. Verification of Spectrochemical series.
10. Preparation of acetylacetonato complex of Cu^{2+} and Fe^{3+} . Determine λ_{max} of the complex.
11. Synthesis of ammine complex of Ni^{2+} and its ligand exchange reaction such as acetylacetone, DMG, glycine by substitution method.

Essential/recommended readings

Theory:

1. Huheey, J. E.; Keiter, E.A.; Keiter, R. L.; Medhi, O.K. (2009), **Inorganic Chemistry- Principles of Structure and Reactivity**, Pearson Education.
2. Cotton, F.A.; Wilkinson, G. (1999), **Advanced Inorganic Chemistry**, Wiley-

- VCR.
3. Miessler, G.L.; Fischer P.J.; Tarr, D. A. (2014), **Inorganic Chemistry**, 5th Edition, Pearson.
 4. B.E. Douglas, D.H. McDaniel and J.J. Alexander, **Concepts and Models of Inorganic Chemistry**, JohnWiley,1993, 3rd ed.

Practicals:

1. Jeffery, G.H.; Bassett, J.; Mendham, J.; Denney, R.C. {1989}, **Vogel's Textbook of Quantitative Chemical Analysis**, John Wiley and Sons,
2. Harris, D. C.; Lucy, C. A. {2016}, **Quantitative Chemical Analysis**, 9th Edition, Freeman and Company.
3. Day, R. A.; Underwood, A. L. {2012}, **Quantitative Analysis**, Sixth Edition, PHI Learning Private Limited.

Assessment Methods: All examination and assessments methods shall be in line with the University of Delhi guidelines issued from time to time.

**List of Instruments/Software required for Implementation of Fourth year Course of
Study for each College**

1. UV- Vis Spectrophotometer
2. Table top IR Spectrophotometer
3. ChemDraw, GaussView6/ GaussView5 and Gaussian 16/Gaussian 09 Software
4. Access to p-XRD NMR Spectrophotometer in Department of Chemistry/USIC
5. Rota Evaporator
6. Sonicator
7. Cyclic Voltammeter/ Potentiostat-Galvanostat