K.L.University
Vaddeswaram- 522502
M.Sc., PHYSICAL Chemistry, II-Semester, 2016-17

Course Handout

1. Course Name : Physical Chemistry

2. Course Code : 16CY 1207

3. Course Coordinator : Dr. Anindita Chatterjee

4. Course Structure(LTP) :

L	T	P
4	0	6

5. Credits : 7

6. Team Members : Dr. Anna Venkateswara Rao

Course Description: This course is made to provide a basic understanding in physical chemistry along with recent advances and discoveries of analyzing molecular structure and application of electrochemistry in energy devices and understanding the chemical reaction involved in production of electricity. The students will be enlightened with the principles and important laws of physical chemistry, chemical analysis and estimation of a compound. Develop skills in applications of physical chemistry in designing batteries, photovoltaic devices and fuel cells. They will be able to take challenges in designing new methodologies of analysis and learn about writing laboratory reports. Overall improvement in communication skills will make them successful in their carrier goals.

7. Course Objectives:

Provide in-depth understanding on the physical chemistry method for structure determination of chemical substances using few spectroscopic techniques .To gain fundamental knowledge in electrochemistry and its application in construction of energy devices. Analytical skill development for their future career in both research and industry.

8. Upon completion of the course, students will:

CO	CO	BTL
I	Physical methods of molecular structure determination.	2
II	Application of Electron Spin Resonance spectroscopy.	2
III	Discuss fundamental aspect of electrochemistry for energy device application.	2
IV	Electrochemistry of electrode electrolyte interface	2
V	An ability to analyze, generate experimental skills towards the industrial applications.	2

9. Course outcome Indicators:

CO#	COI-1	COI-2	COI-3
CO-I	Understand the magnetic properties of molecules.	Discuss the principal and theory of NMR Spectroscopy	Application of NMR to structure elucidation
CO-II	Understand the principal of electron spin Resonance	Describe the experimental technique of ESR and g-factor	Application of ESR studies to structure elucidation of free radicals and metal complexes
CO-III	Apply the concept of Electrode potential and redox equilibrium to the analysis and design of electrochemical cells	Understand the concept of concentration cell	Apply redox chemistry and its role in storage devices (batteries) and fuel cells
CO-IV	Explain the unique properties at the electrode electrolyte interface.	Explain charge transfer reaction at the electrode electrolyte interface.	Application of electrochemistry in cyclic voltametry
CO-V	Perform laboratory experiments some physical parameters .	Ability to design and conduct experiments, as well as to organize, analyze and interpret data.	

10. Program Outcomes (Pos):

PO1. Apply knowledge of mathematics, science, engineering fundamentals and an engineering specialization to the conceptualization of engineering models.

PO2. Identify, formulate, research literature and solve complex engineering problems reaching sustained conclusions using first principles of mathematics and engineering sciences.

PO3. Design solutions for complex engineering problems and design systems, components or processes that meet specified needs with appropriate consideration for public health and safety, cultural, societal and environmental considerations.

PO4. Conduct investigations of complex problems including design of experiments, analysis and interpretation of data and synthesis of information to provide valid conclusions.

PO5. Create, select and apply appropriate techniques, resources and modern engineering tools including predictions and modeling, to complex engineering activities, with an understanding of the limitations.

PO6. Function effectively as an individual, and as a member or leader in diverse teams and in multi disciplinary settings.

PO7. Communicate effectively on complex engineering activities with the engineering community and with society at large, such as being able to comprehend and write effective report and design documentation, make effective presentation, give and receive clear instructions.
PO8. Demonstrate understanding of societal, health, safety, legal and cultural issues and the consequent responsibilities relevant to engineering practice.

PO9. Understand and commit to professional ethics and responsibilities and norms of engineering practice.

PO10. Understand impact of engineering solutions in a societal context and demonstrate knowledge of and need for sustainable development.

PO11. Demonstrate a knowledge and understanding of management and business practice, such as risk and change management, and understand their limitations.

PO12. Recognize the need for, and have the ability to engage in independent and lifelong learning.

11. Mapping of Course Objectives with Programme Outcomes:

1. Highest 2. Moderate 3. Use

Programme Outcomes (Pos)												
Course Out come	**P01**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**	**PO11**	**PO12**
CO-I		1	1	1	2	1	2		1		3	1
CO-II		1	1	1	2	1	2		1		3	1
CO-III		1	1	1	2	1	2		1		2	1
CO-IV		2							2			
CO-V			1	1	1	1						

12. Time Table:

Day/Time	9.00-9.50	9.50-10.40	10.50-11.40	11.50-12.40	01:00 -04:00
Monday	Dr. AVR				Physical Chemistry Lab (Dr. AV R)
Tuesday	Dr. AVR				Physical Chemistry Lab (Dr. AC)
Wednesday					
Thursday					

Friday		Dr. AC			
Saturday		Dr. AC			

13. Syllabus:

Physical Chemistry:

CO-I: Nuclear Magnetic Resonance Spectroscopy

Physical methods of molecular structural elucidation: Magnetic properties of molecules-theories of magnetic susceptibility- measurement of magnetic susceptibility. Principle and theory of NMR spectroscopy, Nature of spinning particle and its interaction with magnetic field. Chemical shift and its origin. Spin-Spin interaction-experimental methods. Application of NMR to structural elucidation- Structure of ethanol, dimethylformamide, styrene and acetophenone.

CO-II : **Electron Spin Resonance::**

Principle and experimental technique- g-factor, line shapes and line widths- hyperfine interactions- applications of ESR studies to the structure of free radicals, metal complexes and biological systems.

CO-III: Electrochemistry I:

Electrochemical cell- Galvanic and electrolytic cell. Concentration cell with and without transference- effect of complexation on redox potential- ferricyanide/ferrocyanide couple, Iron(III) phenonthroline/ Iron(II) phenonthroline couple. Determination of standard potential. Activity coefficient from EMF data. Primary and secondary cells, batteries examples. Fuel cells.

CO-IV: Electrochemistry II:

The electrode-electrolyte interface. The electrical double layer. The Helmholtz-Perrin parallel-plate model, the Gouy-Chapman diffuse-charge model and the Stern model. Electrodics: Charge transfer reactions at the electrode-electrolyte interface.Exchange current density and overpotential. Derivation of Butler-Volmer equation. High field approximation, Tafel equation, Low field equilibrium, Nernest equation. Voltametry-Concentration polarization, experimental techniques

CO-V: LAB COMPONENT:

List of Regular Experiments

1. Determination of rate constant of the oxidation of iodide ion with persulphate ion.
2. Relative strengths of acids by studying the hydrolysis of ethylacetate / methyl acetate.

3. Determination of equilibrium constant of $KI_3 \leftrightarrow KI + I_2$ by partition coefficient method and determination of unknown concentration of potassium iodide.
4. Distribution coefficient of Benzoic acid between Benzene and water.
5. Determination of critical solution temperature of phenol-water system Study of the effect of eletrolyteon the miscibility of phenol-water system

Books Suggested:

1. Physical Chemistry by Peter Atkins and Julio de Paula, Oxford University Press.
2. Physical Chemistry by G.W. Castellon, Narosha Publishing House
3. Physical chemistry by K.L. Kapoor

REFERENCE BOOKS:

1. Introduction to Electrochemistry, S.Glasstone.
2. Fundamentals of Molecular Spectroscopy, Banwell
3. Spectroscopy by Barrow.

14. Self Learning Topics:

CO	Topic	Source
I	Chemical Shift	T-1
II	Hyperfine interaction	T-1
III	Characteristics properties of battery	T-1
IV	Structure determination of molecules By NMR and ESR	Internet Sources
V	Basic lab experimental procedure	Internet Sources

15. Session / Lesson Plan

S. No	CO	Session	Content and Source	Learning objective, End of the session student will	Teaching Methodology	Faculty Approach	Student Approach	Cognitive level expected
1	I	1	Introduction to physical Chemistry –II topics	Understand the necessity	Oral	Explanation	Listens and participate	Understand
2	I	2	Magnetic properties of molecule.	Understand	Chalk and talk	Explanation	Listens and participate	Understand
3	I	3	Theory of Magnetic Susceptibility.	Understand	Chalk and talk	Explanation	Listen	Understand
4	I	4	Measurement of magnetic susceptibility	Apply and use	Chalk and talk	Explanation	Listen and Practice	Understand And apply
5	I	5	Principle of NMR Spectroscopy	Understand	Chalk and talk	Explanation	Listen and Practice	Understand And apply
6	I	6	Theory of NMR	Understand	Chalk and talk	Explanation	Listen and	Understand

			Spectroscopy.					
7	I	7	Nature of spinning particles and its interaction with magnetic field.	Understand	Chalk and talk	Explanation	Listen	Understand
8	I	8	Chemical shift and its origin.	Understand	Chalk and talk	Explanation	Listen	Understand
9	I	9	Spin Spin interaction-exerimental methods.	Understand	PPT	Explanation	Listen	Understand
10	I	10	Structure elucidation of ethanol	Apply and use	PPT	Explanation	Listen	Apply and use
11	I	11	Structure elucidation of Dimethylformamide.	Apply and use	Chalk and talk	Explanation	Listen and practice	Apply and use
12	I	12	Structure elucidation of styrene and acetophenone	Apply and use	Chalk and talk /PPT	Explanation	Listen	Apply and use
13	II	13	Introduction toElectron Spin resonance	Understand	Chalk and talk / PPT	Explanation	Listen and analyze	Understand
14	II	14	Principle to Electron Spin resonance	Understand	Chalk and talk	Explanation	Listen	Understand
15	II	15	Exerimental technique to Electron Spin resonance	Understand	Chalk and talk	Explanation	Listen	Understand And remember
16	II	16	Description of g-Fator, line shapes and line widths-hyperfine interaction	Understand	Chalk and talk	Explanation	Listen	Understand And remember
17	II	17	Application of ESR studies to the structure determination of free radicals	Analyze	Chalk and talk /PPT	Explanation	Listen and practice	Analyze
18	II	18	Structure determination of Metal complexes and biological systems.	Analyze	Chalk and talk	Explanation	Listen and practice	Analyze
19	II	19	Introduction to Electrochemistry, Electrode potential	Understand, Analyze	Chalk and talk	Explanation	Listen and practice	Understand and Analyze
20	II	20	Measurement of Electrode potential ,Electrochemical series	Understand, Analyze	Chalk and talk	Explanation	Listen and practice	Understand and Analyze
21	III	21	Electrochemical Cells, Types of electrochemical cells, Concentration Cells	Understand	Chalk and talk / PPT	Explanation	Listen	Understand
22	III	22	Concentration Cells with and without transference	Understand	Chalk and talk	Explanation	Listen and practice	Understand and Analyze
23	III	23	Effect of complexation on redox potential	Analyze	Chalk and talk	Explanation	Listen and practice	Analyze
24	III	24	Ferricyanide/Ferrocyanide coule, Iron(III) phenthroline/ Iron(II) phenthroline couple	Analyze	Chalk and talk	Explanation	Listen	Analyze

25	III	25	Determination of standard potential.	Apply and use	Chalk and talk / PPT	Explanation	Listen	Apply and use
26	III	26	Determination of activity coefficient from EMF data.	Apply and use	Chalk and talk / PPT	Explanation	Listen	Apply and use
27	III	27	Definition of Primary and Secondary cells.	Understand	Chalk and talk	Explanation	Listen and participate	Understand
28	III	28	Chemistry of batteries	Apply and use	Chalk and talk	Explanation	Listen and participate	Apply and use
29	III	29	Explanation of Fuel cell	Apply and use	Chalk and talk	Explanation	Listen	Apply and use
30	III	30	Concept of electrode electrolyte interface, electrical double layer	Understand	Chalk and talk	Explanation	Listen and participate	Understand
31	IV	31	Explanation of Helmholtz-perrin parallel –plate model.	Understand	Chalk and talk	Explanation	Listen	Understand
32	IV	32	Gouy-Chapman diffuse – charge model and stern model	Understand	Chalk and talk	Explanation	Listen	Understand
33	IV	33	Discuss Electrodics: Charge transfer at the interface	Understand	Chalk and talk	Explanation	Listen	Understand
34	IV	34	Explanation of exchange current density and overpotential	Understand	Chalk and talk / PPT	Explanation	Listen	Understand
35	IV	35	Derivation of Butler - Volmer Equation.	Understand	Chalk and talk	Explanation	Listen	Understand
36	IV	36	Understand Highfield concentration.	Understand	Chalk and talk / PPT	Explanation	Listen	Understand
37	IV	37	Explain Polarization effect.	Analyze	Chalk and talk	Explanation	Listen	Analyze
38	1V	38	Derivation of Tafel equation, low field equilibrium	Understand	Chalk and talk	Explanation	Listen and participate	Understand
39	1V	39	Nernst equation, Voltametry	Analyze	Chalk and talk	Explanation	Listen	Analyze
40	IV	40	Concentration polarization, experimental techniques.	Analyze	PPT	Explanation	Listen	Analyze

16. Evaluation scheme:

EVALUATION PLAN FOR COURSES (16CY110-organic chemistry)

Evaluation Component	Marks	Weightage	Date	Duration (Hours)	CO 1		CO 2		CO 3		CO 4		CO-5
	Course Outcome Indicator Number				1	2	1	2	1	2	1	2	
	Blooms Taxonomy Level				1	2	2	2	2	2	1	2	
Assignment Test	20	2.5 %		1 ½	10	10							
Test 1	20	15%*		1 ½			10	10					
Test 2	20			1 ½					10	10			
Home Assignment	20	2.5%		-							10	10	
Quiz	20	2.5%		20 min	5		5		5		5		
Lab	50	12.5%		3 Hrs Continuous Evaluation-15 marks, Viva-vove-10, Test -25. Total marks will be scaled to 5%.									
Attendance	5	5%	----	75% of Theory+25% of lab attendance.									
Semester End Exam	60	35%		3	2	10.5	2	10.5	2	10.5	2	10.5	
	Question Number				3	12	3	12	3	12	3	12	
End-Lab Exam	60	25%			Lab exam will be conducted for 60 marks and scaled to 10%. Initial rubrics for evaluation are: [Record (10) + Write up (10) + Experimentation (25) + Viva-voce(15)].								

*** 75 % of the Best and 25% of other test together will be taken for 20 marks, internal.**

TEST PATERN:

1. **Assignment Test**: 6 Questions will be given in advance and any two questions of the Faculty choice have to be answered.

2. **TEST1 & 2**: It comprises two sections: **Section-1**: 6 short answer question of 1 mark each are to be answered (no choice). **Section-2**: 2 questions of 7 marks each out of 3 questions have to be answered, totaling to 20 marks. **75 % of the Best and 25% of other test together will be taken for 15 marks, internal.**

3. **Home Assignment**: Two Questions will be given for 20 marks each and to be submitted on or before submission date announced by the faculty in the class.

4. **Quiz:** 20 Objective Questions will be given for 20 marks and to be answered in 20 minutes.

5. **Semester End exam**: Four questions with internal choice 4x15=60

Chamber consultation hours: Thursday: 12:40 PM- 2:20PM

Friday: 12:40 PM- 2:20PM

17. Notices:

All notices regarding course matters will be displayed in e-learning site & copy of it in department notice board.

Note:

a. Each student is required to attend all classes regularly with calculator and is required to complete all the work assigned for the course.
b. Instructors of courses are not obligated to provide make-up opportunities for students who are absent, unless the absence has been officially approved. An officially approved absence, however, merely gives the individual who missed the class an opportunity to make up the work and in no way excuses him from the work.
c. Re conduction of tests will not be entertained, whatever may be the reason. Submission of home assignments after the deadline will not be either accepted or awarded any marks.
d. All students in the class must treat others with civility and respect and conduct themselves during class sessions in a way that does not unreasonably interfere with the opportunity of other students to learn. Failure to comply with this requirement may result in points being deducted from a student's final numerical average / soft skills.

18. Signature of the Course Coordinator:

19. Signature of the Group Head:

20. Signature of the HOD: