### **હેમચંદ્રાચાર્ય ઉત્તર ગુજરાત યુનિવર્સિટી** NAAC A (3.02) State University પો.બો.નં.-૨૧, યુનિવર્સિટી રોડ, પાટણ (ઉ.ગુ.) ૩૮૪૨૬૫ ફોનઃ(૦ર૭૬૬) ૨૨૨૭૪૫, ૨૩૦૫૨૯, ૨૩૦૭૪૩, ૨૩૩૬૪૮ Email : regi@ngu.ac.in પરિપત્ર ક્રમાંક – ૪૪ / ૨૦૧૯

વિષયઃ વિજ્ઞાન વિદ્યાશાખાના અનુસ્નાતક કક્ષાના સેમેસ્ટર-૧ થી સેમેસ્ટર-૪ સુધીના નવા અભ્યાસક્રમોનું માળખું તેમજ નવા અભ્યાસક્રમ અંગે...

આ યુનિવર્સિટીના વિજ્ઞાન વિદ્યાશાખા અંતર્ગત વિષયોના અનુસ્નાતક વિભાગો તથા સંલગ્ન વિજ્ઞાન વિદ્યાશાખાની તમામ કોલેજોના આચાર્યશ્રીઓને જણાવવાનું કે, એકેડેમીક કાઉન્સિલ ની તા. ૫/*૬*/૨૦૧૮ ની સભા ના નિર્દિષ્ટ ઠરાવો અન્વયે UGC ની Model curriculum અંગેની Guideline સંદર્ભે વિજ્ઞાન વિદ્યાશાખા હેઠળના નીચેના વિષયોના અનુસ્નાતક કક્ષાના સામેલ પરિશિષ્ટ પ્રમાણેના નવા અભ્યાસક્રમનું માળખું તેમજ અભ્યાસક્રમો <u>શૈક્ષણિક</u> <u>વર્ષ: ૨૦૧૯–૨૦ થી ક્રમશ: અમલ માં આવે તે રીતે</u> મંજૂર કરેલ છે. જેનો અમલ કરવા સારૂ સબંધિતોને આ સાથે તોકલવામાં આવે છે.

N/	ક્રમ નં.	અભ્યાસક્રમ	એકેડેમીક કાઉન્સિલની તારીખ:૦૫/૦૬/૨૦૧૮ના ઠરાવ ક્રમાંક	સેમેસ્ટર
2141 June on	2	અભ્યાસક્રમો નું માળખું	09	તમામ સેમેસ્ટર
Whist white	2	રસાયણશાસ્ત્ર	88	સેમ૧ થી સેમર
	3	પ્રાણીશાસ્ત્ર	૪૫	સેમ.– ૧થી સેમ.–૪
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460314	9	ભૌતિકશાસ્ત્ર	ųo	સેમ૧ થી સેમ૪

આ બાબતની સબંધિત અધ્યાપકો તથા વિધાર્થીઓને આપના સ્તરેથી જાણ કરવા વિનંતી છે.

નોંધ :- (૧) વિદ્યાર્થીઓની જરૂરીયાત માટે પરિપત્રની એક નકલ કોલેજના ગ્રંથાલયમાં મૂકવાની રહેશે.

(૨) આ અભ્યાસક્રમ / સ્ક્રીમ યુનિવર્સિટીની વેબ સાઈટ <u>www.ngu.ac.in</u> ૫૨ પણ ઉપલબ્ધ કરાવવામાં આવન્ન જેછે.

60000 કલસચિવવતી

બિકાશ : ઉપર મુજબ

નં.-એક/અ×સ/ ૧૦૧૬૩ /૨૦૧૯ તારીખ: ૧૪/૦૩/૨૦૧૯

પ્રતિ,

૧. અધ્યક્ષશ્રી/ કો.ઓર્ડીનેટ૨શ્રી–વિજ્ઞાન વિદ્યાશાખા અંતર્ગત વિષયોના અનુસ્નાતક વિભાગો, હેમ. ઉ.ગુ. યુનિવર્સિટી, પાટણ.

ર. સંલગ્ન સાયન્સ કોલેજોના આચાર્યશ્રીઓ

૩. ર્કા. એમ. બી. પ્રજાપતિ (ડીનશ્રી),ગણિતશાસ્ત્ર ભવન, હેમ. ઉ.ગુ. યુનિવર્સિટી, પાટળ.

૪. પરીક્ષા નિયામકશ્રી, હેમચંદ્રાચાર્ય ઉત્તર ગુજરાત યુનિવર્શિટી, <u>પાટલ.</u> (પાંચ નકલ)

પ. ગ્રંથપાલશ્રી, હેમ.ઉત્તર ગુજરાત યુનિવર્સિટી, <u>પાટલ</u> (વિદ્યાર્થીઓના ઉપયોગ સારૂ રેકર્ડ ફાઈલ માટે)

૬. સિસ્ટમ એનાલીસ્ટશ્રી, કોમ્પ્યુટર (રીઝલ્ટ) સેન્ટર, હેમ.ઉ.ગુ.યુનિવર્સિટી, <u>પાટલ.</u> તરક પરિણામ માટે તથા વેબસાઈટ પર મૂકવા સારૂ.

૭. માન.કુલપતિશ્રી/ કુલસચિવશ્રીનું કાર્યાલય, હેમ.ઉત્તર ગુજરાત યુનિવર્સિટી, <u>પાટણ.</u>

૮. અનુસ્નાતક પ્રશાખા (એકેડેમીક શાખા) હેમચંદ્રાચાર્ય ઉત્તર ગુજરાત યુનિવર્સિટી, પાટળ.

૯. મુખ્ય હિસાબી અધિકારીશ્રી (મહેકમ), હેમચંદ્રાચાર્ય ઉત્તર ગુજરાત યુનિવર્સિટી, પાટણ તરફ → પરિપત્રની ફાઈલ અર્થે

૧૦. સિલેકટ ફાઈલે. (૨ નકલ્ર)



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### Hemchandracharya North Gujarat University

Accredited by NAAC with "A" Grade (CGPA 3.02)

P.Box. No.21, University Road, Patan (N.G.), 384 265

Phone : (02766) 222745, 230529, 230743, 233648 Email : regi@ngu.ac.in Fax : (02766) 231917 Website : www.ngu.ac.in

The Proposed New Structure for M.Sc. Course is based on choice Based Credit System (CBCS) which is in force from June – 2018

#### **CBCS** Course Pattern

- 1. This programme is divided into four Semesters (Two Years). The duration of an academic year consists of two semesters, each of 15 weeks for teaching. The academic session in each semester will provide 90 teaching days. 24 credit each year X 4 semester= 96 credits master level.
  - There will be three categories of courses / papers in this programme :
    - A. Four Compulsory Core theory courses with 4 credits each in each semester.
    - B. One Choice Based Elective Course (disciplinary / interdisciplinary) with 2 credits in each semester.
    - C. Two Practical's each of Three credits in each semesters .
    - D. In the IV Semester as above a,b,c or instead of above A,B, C ; a student can undertake Three core theory courses (12 credits) and project / field work (12 credits), OR Major Dissertation (24 credits) OR as per decided by BOS.
- 3. Detailed Course Pattern for each Semester is given bellow.

Course	Name of the Course	Exam. Duration (Hours)	Ext. Marks	Int. Marks	Total Marks	Teach, Hours Per week	Credit point
Paper - I	Core-I	2:30	70	30	100	4	4
Paper – II	Core-II	2:30	70	30	100	4	4
Paper – III	Core-III	2:30	70	30	100	4	4
Paper – IV	Core-IV	2:30	70	30	100	4	4
Practical : Paper – I	Pract-I	3/4	75		75	6	3
Practical : Paper – II	Pract-II	3/4	75		75	6	3
Elective Course (Any One) Disciplinary / Interdisciplinary		2:00	50		50	2	2
TOTAL			480	120	600	30	24

#### M.Sc. : Semester - I

### M.Sc. : Semester - II

Course	Name of the Course	Exam. Duration (Hours)	Ext. Marks	lnt. Marks	Total Marks	Teach, Hours Per week	Credit point
Paper – V	Core-V	2:30	70	30	100	4	4
Paper – VI	Core-VI	2:30	70	30	100	4	4
Paper – VII	Core-VII	2:30	70	30	100		
Paper – VIII	Core-VIII	2:30	70	30	100	4	4
Practical : Paper - III	Pract-III	3/4	75	50		4	4
Practical : Paper – IV	Pract-IV	3/4			75	6	3
Elective Course (Any One)	ridceiv		75		75	6	3
Disciplinary / Interdisciplinary		2:00	.50		50	2	2
TOTAL			480	120	600	30	24

### M.Sc. : Semester - III

Course .	Name of the Course	Exam. Duration (Hours)	Ext. Marks	lnt. Marks	Total Marks	Teach, Hours Per week	Credit point
Paper – IX	Core-IX	2:30	70	30	100	4	4
Paper – X	Core-X	2:30	70	30	100	4	4
Paper XI	Core-XI	2:30	70	30	100	4	4
Paper – XII	Core-XII	2:30	70	30	100	4	4
Practical : Paper – V	Pract-V	3/4	75		75	6	3
Practical : Paper – VI	Pract-VI	3/4	75		75	6	3
Elective Course (Any One) Disciplinary / Interdisciplinary		2:00	50		50	2	2
TOTAL			480	120	600	30	24

### M.Sc. : Semester - IV

14.52

Course	Name of the Course	Exam. Duration (Hours)	Ext. Marks	Int. Marks	Total Marks	Teach, Hours Per week	Credit point
Paper – XIII	Core-XIII	2:30	.70	30	100	4	4
Paper – XIV	Core-XIV	2:30	70	30	100	4	4
Paper – XV	Core-XV	2:30	70	30	100	4	4
Paper – XVI	Core -XVI	2:30	70	30	100	4	4
Practical : Paper – VII	Pract-VII	3/4	75		75	6	3
Practical : Paper – VIII	Pract-VIII	3/4	75		75	6	3
Elective Course (Any One) Disciplinary / Interdisciplinary		2:00	50		50	2	2
TOTAL			480	120	600	30	24

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Course	Name of the Course	Exam. Duration (Hours)	Ext. Marks	Int. Marks	Total Marks	Teach, Hours Per week	Credit point
Paper – XIII	Core-XIII	2:30	70	30	100	4	4
Paper – XIV	Core-XIV	2:30	70	30	100	4	4
Paper – XV	Core-XV	2:30	70	30	100	4	4
Major Dissertation			210	90	300	18	12
TOTAL			420	180	600	30	24

NOTE :

- 1. For 4 credit course: Each syllabus is of 4 Units having equal weightage.
- 2. For 2 credit course: Each syllabus is of 2 Units having equal weightage.
- 3. There is no section in semester end examinations i.e. questions Paper is without sections.
- For question paper of 70 marks: Each Question paper contains 4 questions: Q-1 from unit-I of 18 marks, Q-2 from unit-II of 17 marks, Q-3 from unit-III of 18 marks and last Q-4 from unit-Iv of 17 marks from entire course.
- 5. For question paper of 50 marks: Each Question paper contains 3 questions: Q-1 from unit-I of 20 marks, Q-2 from unit-II of 20 marks, and last Q-3 is of objective types having 10 marks from entire course.

[BOS may add some specifications with reference to above structure.]



# HEMCHANDRACHRAYA NORTH GUJARAT UNIVERSITY

NAAC A (3.02) State University PATAN - 384265

## **Faculty of Science**

### M.Sc.-Chemistry

Syllabus/Scheme

### Sem – 1 & 2

Sem / CBCS / Grading Pattern

W.E.F. June -2019 (and thereafter)

DATE: 05/06/2018

TOTAL PAGE-41

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### CURRICULUM Hemchandracharya North Gujarat University, Patan. M.Sc. (Chemistry) (WEF June: 2018) 2019 <u>General Information of Semester I &II</u> <u>Syllabus According To CBCS Pattern</u>

- 1. The medium of instruction, question papers as well as answers in examinations will be English only.
- Passing standard: 40% As per the revised rules and regulation of Hemchandracharya North Gujarat University, Patan. (Aca/Axs/744/2018, Date 27/4/2018)
- 3. Viva voce will be pertaining to practicals.
- 4. The degree will be awarded in M.Sc. (Chemistry) in specialized branch.
- 5. The result sheet of all semesters will contain the name of elective papers selected by the candidate, the grade and the credit secured.
- 6. A maximum of 10% students passing second semester may be allowed for dissertation at the 4<sup>th</sup> semester. Such students will be exempted from practical as well as viva of fourth semester, in lieu of that the dissertation of candidate will be assessed with 100 marks of dissertation and 50 marks of the viva of dissertation.

If the number of students willing to opt dissertation exceeds 10%, dissertation will be given on the basis of merit of combined marks of first and second semester. The dissertation will be allotted to the students in the beginning of third semester by head of the department/ P.G. Center.

 Intake of students every center 25 (organic branch) 15 for Inorganic & physical branch, University Department. 55 (Inorganic, Organic and Physicalbranches) 8. For semester, I & II

The internal evaluation for total 90 marks will be done as per the continuous evaluation process as under.

	Marks
) Weekly test of theory (minimum 6)	56
) Internal Practical examination (once a semester)	20
	14
) Problem Solving / New Practical	06
) Book review (In students own hand writing, separate book for all)	07
	07
	<u>10</u>
Total	120
	<ul> <li>Weekly test of theory (minimum 6)</li> <li>Internal Practical examination (once a semester)</li> <li>Students seminar (Once a Semester)</li> <li>Problem Solving / New Practical</li> <li>Book review (In students own hand writing, separate book for all)</li> <li>Project work assessment (separate for all)</li> <li>Quiz / Questionnaire</li> </ul>

9. A batch of Chemistry Practical will consist of 20 students per teacher.

 For semester I, the paper, CHNN-401, CHNN-402, CHNN-403, CHNN-404 are compulsory. Furthermore, students will have choice to select any one of CHNN-405 A or CHNN-405 B.

- For semester II, the papers, CHNN-501, CHNN-502, CHNN-503, and CHNN-504 are compulsory. In addition, the student has a choice to select either CHNN-505 A or CHNN-505 B.
- 12. For all the semesters, the total marks will be given out of 600. The cumulative grade will be as per university rules.

# Note: During the preparation of this curriculum, ample care is taken for consideration of the followings:

- A. Model curriculum of U.G.C.
- B. Concept of continuous evaluation
- C. CGPA (Cumulative Grade Point Average Credit)
- D. CBCS (Choice Based Credit System)
- E. Semester approach
- F. Revised rules and regulation of Hemchandracharya North Gujarat University, Patan.
- G. NET (NATIONAL ELIGIBILITY TEST) curriculum
- For university Examination for each batch, maximum 30 students / three examiners / 3 days.

One day each for Inorganic, Organic and Physical chemistry branch, Marks will be 50 from each branch and hence total practical marks will be 150 (including viva), for CHNN- 406 and CHNN-407 for semester I. Similar pattern will be for MSc. semester II.

### Hemchandracharya North Gujarat University, Patan. M.Sc. (Chemistry) (WEF June: 2018) 2019 <u>Semester and Examination</u> <u>Semester – I</u>

Work Load	Paper No.	Subject	External Marks	Internal Marks	Credit
60 Hrs.	CHNN-401	Inorganic Chemistry	70	30	4
60 Hrs.	CHNN-402	Organic Chemistry	70	30	4
60 Hrs.	CHNN-403	Physical Chemistry	70	30	4
60 Hrs.	CHNN-404	Group Theory, Spectroscopy and Diffraction Method	70	30	4
30 Hrs	CHNN-405 A	Computers for Chemists	50		2
30 Hrs	CHNN-405 B	Computational Chemistry	50		2
00 Hrs.	CHNN-406	Practical I	75 *		3
0 Hrs.	CHNN-407	Practical II	75 *		3
	Total		480	120	24

\*Each CHNN-406 and CHNN – 407 includes 15 marks of viva in the total of 75 marks of viva voce examination.

Working per semester minimum 90 days (15weeks)

### Hemchandracharya North Gujarat University, Patan. M.Sc. (Chemistry) (WEF June: 2<del>018</del>)2019 <u>Semester and Examination</u> Semester - II

Work	Paper No.	Subject	External	Internal	Credit
Load			Marks	Marks	
60 Hrs.	CHNN-501	Inorganic Chemistry	70	30	4
60 Hrs.	CHNN-502	Organic Chemistry	70	30	4
60 Hrs.	CHNN-503	Physical Chemistry	70	30	4
60 Hrs.	CHNN-504	Spectroscopy – part II	70	30	4
30 Hrs	CHNN-505 A	Organotransition Metal Chemistry	50		2
30 Hrs	CHNN-505 B	Bioinorganic and Supramolecular Chemistry	50		2
90 Hrs.	CHNN-506	Practical I	75 *		3
90 Hrs.	CHNN-507	Practical II	75 *		3
	Total		480	120	24

\*Each CHNN-506 and CHNN – 507 includes 15 marks of viva in the total of 75 marks of viva voce examination

Working per semester minimum 90 days (15weeks)

# CURRICULUM HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester – 1 Course: CHNN – 401 (Core compulsory)

### **Inorganic Chemistry**

# I Stereochemistry and Bonding in Main Group Compounds

VSEPR, Walsh diagrams (tri- and penta- atomic molecules), d-p,I bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

### II Metal-Ligand Equilibria in Solution

Stepwise and overall formation constants and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH - metry and spectrophotometry.

## **III Reaction Mechanism of Transition Metal Complexes**

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valence bond and crystal field theories, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of the subtitution reaction. Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

**IV Metal-Ligand Bonding** 

16 Hrs

8 Hrs

24 Hrs

12 Hrs

5

# 6

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, n-bonding and molecular orbital theory.

#### **Books Suggested**

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.

2. Inorganic Chemistry, J.E. Huhey, Harpes&Row.~

3. Chemistry of the Elements, vN.N. Greenwood and A. Earnshow, Pergamon.

4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.

5. Magnetochemistry, FI.L. Carlin, Springer Verlag.

6. Comprehensive Coordination Chemistry eds., G. Wilkinson, FLD. Gillars and J.A McCleverty, Pergamon.

### CURRICULUM

### HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester - 1

### Course: CHNN – 402 (Core compulsory)

### **Organic Chemistry**

### I Nature of Bonding in Organic Molecules

Delocalized chemical bonding—conjugation, cross conjugation, resonance, hyperconjugation, bonding in fullerenes, tautomerism.

Aromaticity in benzenoid and non-benzenoid compounds, alternant and non-alternant hydrocarbons, Huckel's rule, energy level of pi-molecular orbitals, annulenes, anti— aromaticity, w-aromaticity, homo-aromaticity, PMO approach.

Bonds weaker than covalent- addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

#### **II Stereochemistry**

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity,

conformation of sugars, steric strain due to unavoidable crowding.

Elements of symmetry, chirality, molecules with more than one chiral center, threo and

erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic

atoms, groups and faces, stereospecific and stereoselective synthesis. Asymmetric

synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and

spiranes), chirality due to helical shape.

Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus.

7

15 Hrs

10 Hrs

#### **III Reaction Mechanism: Structure and Reactivity**

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Hard and soft acids and bases.

Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes.

Effect of structure on reactivity - resonance and field effects, steric effect, quantitative treatment. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

#### IV (A) Aliphatic Nucleophilic Substitution

The SN2, SN1, mixed SN1 and SN2 and SET mechanisms.

The neighbouring group mechanism, neighbouring group participation by Pi and sigma bonds, anchimeric assistance.

Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations.

The SNi mechanism.

Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambidentnucleOphile, regioselectivity.

#### (B) Free Radical Reactions

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic

15 Hrs

substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity.

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

#### **Books Suggested**

- Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.
- 2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- 4. Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
- 5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
- 6. Modern Organic Reactions, H. O. House, Benjamin.
- Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
- 8. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.

9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.

10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.

11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

#### CURRICULUM

### HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester - 1 Course: CHNN – 403 (Core compulsory) Physical Chemistry

#### Unit-I (A) Quantum Chemistry

15 Hrs

15 Hrs

#### Introduction to Exact Quantum Mechanical Results

The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

#### (B) Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (first order and nondegenerate). Applications of variation method and perturbation theory to the Helium atom.

#### Unit-II -(A) Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigenfunctions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

#### (B) Electronic Structure of Atoms

Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the pn configuration, term separation energies for the dn configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self -consistent field, the virial theorem.

10

#### (C) Molecular Orbital Theory

Huckel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, cyclopropenyl radical, cyclobutadiene etc. Introduction to extended Huckel theory.

### Unit-III Thermodynamics

#### **Classical Thermodynamics**

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity.

Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient, Debye—Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic strength.

Application of phase rule to three component systems; second order phase transitions.

### Unit-IV (A) Statistical Thermodynamics

15 Hrs

15 Hrs

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers).

Partition functions - translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition functions. Applications of partition functions.

Heat capacity behaviour of solids — chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac statistics, distribution law and applications to metal.

Bose—Einstein statistics — distribution law and application to helium.

#### (B) Non-Equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equations, microscome reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological systems, coupled reactions.

#### **Books Suggested**

- 1. Physical Chemistry, P.W. Atkins, ELBS.
- 2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
- 3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
- 4. Coulson's Valence, R. McWeeny, ELBS.
- 5. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
- Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
- 7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenun
- 8. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Fteddy, Plenum.
- 9. Introduction to Polymer Science, V.Fl. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

## CURRICULUM HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester - 1 Course: CHNN – 404 (Core compulsory) Group Theory, Spectroscopy and Diffraction Method

### I Symmetry and Group Theory in Chemistry

12 Hrs

10 Hrs

7 Hrs

Symmetry elements and symmetry operation, definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes. Point symmetry group. Schonflies symbols, representations of groups by matrices (representation for the Cn, Cnv, Cnh, Dnh etc. groups to be worked out explicitly). Character of a representation. The great orthogonality theorem (without proof) and its importance. Character tables and their use; spectroscopy. Hybridization for Td and Oh geometries with sigma and pi bonding.

#### Unit-II (A) Unifying Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter—absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

#### II-(B) Microwave Spectroscopy

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

13



#### Unit-III Vibrational Spectroscopy

#### Infrared Spectroscopy

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration—rotation spectroscopy, P,Q,Fi branches. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis.

#### Unit-IV-(A) Raman Spectroscopy

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

#### **(B) OTHER TECHNIQUES**

#### Photoacoustic Spectroscopy

Basic principles of. photoacoustic spectroscopy (PAS), PAS-gases and condensed systems, chemical and surface applications.

#### (C) Electron Diffraction

Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

#### (D) Neutron Diffraction

Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

10 Hrs

3 Hrs

3 Hrs

# 5

#### **Books Suggested**

1. Modern Spectroscopy, J.M. Hollas, John Wiley.

- 2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and FL. Ho, Wiley Interscience.
- 3. NMR, NOR, EPB and Mossbauer Spectroscopy in Inorganic Chemistry, RV. Parish, Ellis Harwood.
- 4. Physical' Methods in Chemistry, FLS. Drago, Saunders College.
- 5. Chemical Applications of Group Theory, F. A. Cotton.
- 6. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
- 7. Basic Principles of Spectroscopy, Ft. Chang, McGraw Hill.
- 8. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
- 9. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
- 10. Introduction to Magnetic Resonance, A Carrington and AD. Maclachalan, Harper & Row.

#### **CURRICULUM**

### HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester - 1 Course: CHNN – 405 (A) (Elective course) **Computers for Chemists**

#### CHNN -405 (A) Computers for Chemists

#### 30 Hrs (2 Hrs/week)

This is a theory-cum-laboratory course with more emphasis on laboratory work.

#### I Introduction to Computers and Computing

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data Processing, principles of programming. Algorithms and flow-charts.

#### **II Computer Programming in FORTRAN/C/BASIC**

(The language features are listed here with reference to FORTRAN. The instructor may choose another language such as BASIC or C and the features may be replaced appropriately). Elements of the computer language. Constants and variables. Operations and symbols. Expressions. Arithmatic assignment statement. Input and Output. Format statement. Termination statements. Branching statements such as IF or GO TO statement. LOGICAL variables. Double precision variables. Subscripted variables and DIMENSION. DO statement. FUNCTION and SUBFIGUTINE. COMMON and DATA statements. (Students learn the programming logic and these language features by 'hands' on' experience on a personal computer from the very beginning of this topic).

16

8 Hrs

10 Hrs

#### **III Programming in Chemistry**

Development of small computer codes involving simple formulae in chemistry, such as van der Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge data base.

#### **Books Suggested**

- 1. Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
- 2. Computational Chemistry, A.C. Norris.
- 3. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.
- 4. Computer Programming in FORTRAN IV, V. Rajaraman, Prentice Hall.
- 5. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.

#### CURRICULUM

#### HEMCHANDRACHARYA

#### NORTH GUJARAT UNIVERSITY, PATAN

#### M.Sc. (Chemistry) Semester - 1

#### Course: CHNN – 405 (B)(Elective course)

#### **Computational Chemistry**

#### I Fortran/C Programming and Numerical Methods

Advanced programming features of FORTRAN/C. Basic theory, discussion of algorithms and errors for the following numerical methods. Examples from chemistry should be selected for illustrating the methods. The teacher may select ANY THREE of the following subtopics considering the background of students, available time etc.

#### a. Solution of Equations

Bisection, regular falsi, Newton ~Fiaphson and related methods for solving polynomial and

transcendental equations. Convergence. Errors and ill-conditioning.

#### **b.** Linear Simultaneous Equations

Gaussian elimination, Gauss -Seidel method, Gauss-Jordan method. Pivoting

strategy. Errors and ill conditioning.

#### c. Eigenvalues and Matrix Diagonalization

Jacobi and Householder methods, analysis or errors.

#### d. Interpolation

Newton forward and backward difference, central differenced formulae. Lagrange and Hermite interpolation. Polynomial wiggle problem.

#### e. Numerical Differentiation

Solution of simple differential equations by Taylor series and Runge-Kutta methods.

#### f. Numerical Integration

Newton-Cotes formulae, Romberg integration, errors in integration formulae.

The students should develop computer programs for some of the above numericalmethods.

15 Hrs

### II Running of Advanced Scientific Packages

The students are expected to get hands on experience of running a few selected advanced level scientific software packages after a brief introduction to the basic theory and methodology. ab initio quantum chemical packages such as GAUSSIAN/GAMES with carefully designed exercises for illustrating various features of the packages.

#### **Books Suggested**

- 1. The Chemistry Mathematics Book, E. Steiner, Oxford University Press.
- 2. Mathematics for Chemistry, Doggett and Sublifte, Longman.
- 3. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
- 4. Chemical Mathematics, D.M. Hirst, Longman.
- 5. Applied Mathematics for Physical Chemistry, JR. Barrante, Prentice Hall.
- 6. Basic Mathematics for Chemists, Tebbutt, Wiley.

#### M.Sc. SEM -1

#### **Practical I**

#### CHNN - 406 (Inorganic + Organic)

#### **Qualitative and Quantitative Analysis**

A. Less common metal ions - Tl, Mo, W, Ti, Zr, Th, V, U (two metal ions in cationic/anionic

forms)

B. Insolubles - oxides, sulphates and halides

#### **Books Suggested**

- Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
- 2. Synthesis and Characterization of inorganic Compounds, W. L. Jolly, Prentice Hall
- 3. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- 4. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- 5. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
- 6. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
- 7. Vogel's Textbook of Practical Organic Chemistry, A. Ft. Tatchell, John Wiley
- 8. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman
- 9. Findley's Practical Physical Chemistry, B. P. Levitt, Longman
- 10. Experimental Physical Chemistry, RC. Das and B. Behera, Tata McGraw Hill.

#### **Organic Synthesis**

Acetylation: Acetylation of cholesterol and separation of cholesteryl acetate by column chromatography

Oxidation: Adipic acid by chromic acid oxidation of cyclohexanol

Grignard reaction: Synthesis of triphenylmethanol from benzoic acid

Aldol condensation: Dibenzal acetone from benzaldehyde

Sandmeyer reaction: p-Chlorotoluene from p-toluidine

Acetoacetic ester Condensation: Synthesis of ethyl-n-butylacetoacetate by A.E.E. condensation.

Cannizzaro reaction: 4-Chlorobenzaldehyde as substrate

Friedel Crafts Reaction: B-Benzoyl pr0pionic acid from succinic anhydride and benzene

Aromatic electrophilic sustitutions: Synthesis of p-nitroaniline and p-bromoaniline

The Products may be Characterized by Spectral Techniques

#### **Quantitative Analysis**

Determination of the percentage or number of hydroxyl groups in an organic compound by

acetylation method

Estimation of amines/phenols using bromate bromide solution/or acetylation method

Determination of Iodine and Saponification values of an oil sample.

Determination of COD of water sample

#### **Books Suggested**

- 1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
- 2. Synthesis and Characterization of inorganic Compounds, W. L. Jolly, Prentice Hall
- Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- 4. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- 5. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
- 6. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
- 7. Vogel's Textbook of Practical Organic Chemistry, A. Ft. Tatchell, John Wiley
- 8. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman
- 9. Findley's Practical Physical Chemistry, B. P. Levitt, Longman

10. Experimental Physical Chemistry, RC. Das and B. Behera, Tata McGraw Hill.

#### SEM-I

#### **Practical** - II

#### CHNN – 407Physical Chemistry

#### Error Analysis and Statistical Data Analysis

Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, student 't' test, null hypothesis, rejection criteria, F & Q test; linear regression analysis, curve fitting.

Calibration of volumetric apparatus, burette, pipette and standard flask.

#### Adsorption

To study surface tension - concentration relationship for solutions (Gibbs equation).

Phase Equilibria

(i) Determination of congruent composition and temperature of a binary system (e.g.,

Diphenylaminen - benzophenone system)

(ii) Determination of glass transition temperature of a given salt (e.g., CaCl2)

conductometrically.

(iii) To construct the phase diagram for three component system (e.g., chloroform—acetic Acid - water).

#### **Chemical Kinetics**

(i) Determination of the effect of (a) Change of temperature (b) Change of concentration of reactants and catalyst and (c) lonic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.

(ii) Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar Media



#### Electrochemistry

#### A. Conductometry

(i) Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically.

(ii) Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO4,

BaSO4) conductometrically.

(iii) Determination of the strength of strong and weak acids in a given mixture conductometrically.

#### Potentiometry/pH metry

I) Determination of strengths of halides in a mixture potentiometrically.

II) Determination of the valency of mercurous ions potentiometrically.

#### Polarimetry

(i) Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.

(ii)Enzyme kinetics - inversion of sucrose

#### **Books Suggested**

- 1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
- 2. Synthesis and Characterization of inorganic Compounds, W. L. Jolly, Prentice Hall
- Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- 4. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- 5. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
- Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.
   Vogel's Taythook of Dravia 10
- 7. Vogel's Textbook of Practical Organic Chemistry, A. Ft. Tatchell, John Wiley
- 8. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman
- 9. Findley's Practical Physical Chemistry, B. P. Levitt, Longman

10. Experimental Physical Chemistry, RC. Das and B. Behera, Tata McGraw Hill.

### CURRICULUM HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester – II Course CHNN – 501 (Core compulsory) Inorganic Chemistry

I Electronic Spectra and Magnetic Properties of Transition Metal Complexes 20 Hrs Spectroscopic ground states, correlation, Orgel and Tanabe-Sugano diagrams for transition metal complexes (dI-d9 states), calculations of Dq, B and [3 parameters, charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover.

#### II Metal Pi-Complexes

Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation, important reactions of metal carbonyls; preparation, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygen complexes; tertiary phosphine as ligand.

#### **III Metal Clusters**

Higher boranes, carboranes, metalloboranes and metallocarboranes. Metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Unit-IV(A)Isopoly and Heteropoly Acids and Salts3 Hrs(B)Sigma bonded organo metallic compounds11 Hrs

of transition metals, classification, synthesis, structure, properties and applications.

14 Hrs

#### **Books Suggested**

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.

2. Inorganic Chemistry, J.E. Huhey, Harpes&Row.~

3. Chemistry of the Elements, vN.N. Greenwood and A. Earnshow, Pergamon.

4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.

5. Magnetochemistry, FI.L. Carlin, Springer Verlag.

6. Comprehensive Coordination Chemistry eds., G. Wilkinson, FLD. Gillars and J.A. McCleverty, Pergamon.

#### CURRICULUM

### HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester – II Course CHNN – 502 (Core compulsory) Organic Chemistry

#### Unit-I (A) Aliphatic Electrophilic Substitution

Bimolecular mechanisms- SE2 and SEi. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

#### (B) Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeir reaction, Gattermann-Koch reaction.

#### Unit-II (A) Aromatic Nucleophilic Substitution

The SNAr, SN1, benzyne and SRN1 mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

#### (B) Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of

5 Hrs

#### 5 Hrs

6 Hrs

aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

#### Unit-III (A) Addition to Carbon-Hetero Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates - Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

Hydrolysis of esters and amides, ammonolysis of esters.

#### (B) Elimination Reactions

The E2, E1 and Ech mechanisms and their spectrum. Orientation of the double bond. Reactivity - effects of substrate structures, attacking base, the leaving group and the medium.

Mechanism and orientation in pyrolytic elimination.

#### Unit-IV Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3- butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward - Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions - conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloaddditions -antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements - suprafacial and antarafacial shifts of H, Sigmatropic shifts involving carbon moieties, 3,3- and 5,5- Sigmatropic rearrangements. Claisen, Cope and aza -Cope rearrangements. Fluxional tautomerism. Ene reaction.

27

20 Hrs

12 Hrs

5 Hrs



#### **Books Suggested**

1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wiley.

21420 Minter

- 2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
- 3. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
- Structure and Mechanism in Organic Chemistry, C. K. Ingold, Cornell University Press.
- 5. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
- 6. Modern Organic Reactions, H. 0. House, Benjamin.
- 7. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
- 8. Pericyclic Reactions, 8. M. Mukherji, Macmillan, India.
- 9. Reaction Mechanism in Organic Chemistry, 8. M. Mukherji and S. P. Singh, Macmillan.
- 10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
- 11. Stereochemistry of Organic Compounds, P.S. Kalsi, New Age International.

## CURRICULUM HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester – II Course CHNN – 503 (Core compulsory) Physical Chemistry

#### Unit-I Chemical Dynamics

#### 20 Hrs

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov -Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann — Hinshelwood and Rice-Ramsperger - KasseI—Marcus [RRKM] theories of unimolecular reactions)

#### Unit-II Surface Chemistry

#### (A) Adsorption

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapour pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface films on liquids (Electro-kinetic

29

12 Hrs



phenomenon), catalytic activity at surfaces.

#### (B) Micelles

Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CMC), factors affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization - phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

#### **Unit-III Macromolecules**

Polymer — definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization.

08 Hrs

20 Hrs

Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

#### Unit-IV Electrochemistry

Electrochemistry of solutions. Debye-Hiickel - Onsager treatment and its extension, ion solvent interactions. Debye-HUckel-Jerum mode. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equations (surface excess), methods of determination. Structure of electrified interfaces. Guoy -Chapman, Stern, Graham — Devanathan — Mottwatts, Tobin, Bockris, Devanathan models.

Over potentials, exchange current density, derivation of Butler -Vo|mer equation, Tafel plot.

Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling.

Semiconductor interfaces — theory of double layer at semiconductor, electrolyte solution interfaces, structure of double layer interfaces. Effect of light at semiconductor solution interface.

Electrocatalysis ----- influence of various parameters. Hydrogen electrode.

30

Bioelectrochemistry, threshold membrane phenomena, Nernst-Planck equation, Hodges -

Huxley equations, core conductor models, electrocardiography.

Polarography theory, llkovic equation; half wave potential and its significance.

Introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring

and prevention methods.

#### **Books Suggested**

- 1. Physical Chemistry, P.W. Atkins, ELBS.
- 2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
- 3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
- 4. Coulson's Valence, R. McWeeny, ELBS.
- 5. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
- 6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
- 7. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenun
- 8. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Fteddy, Plenum.
- Introduction to Polymer Science, V.Fl. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

## CURRICULUM HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester – II Course CHNN – 504 (Core compulsory) Spectroscopy – part II

Unit-I Electronic Spectroscopy		
(A) Atomic Spectroscopy	4 Hrs	No. of
Energies of atomic orbitals, vector representation of momenta and vector coupling,		ľ
spectra of hydrogen atom and alkali metal atoms.		
(B) Molecular Spectroscopy	4Hrs	
Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and		
geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic	2	
molecules. Emission Spectra; radiative and non-radiative decay, internal conversion,		
spectra of transition metal complexes, charge-transfer spectra.		
(C) Photoelectron Spectroscopy	10 Hrs	
Basic principles; photo-electric effect, ionization process, Koopman's theorem.		
Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA.	ę	The second
Auger electron spectroscopy — basic idea.		
Unit-II Magnetic Resonance Spectroscopy	24Hrs	
Nuclear Magnetic Resonance Spectroscopy		
Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift		
and its measurements, factors influencing chemical shift, deshielding, spin-spin		
interactions, factors influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A282		
etc.), spin decoupling; basic ideas about instrument, NMR studies. of nuclei other than		
proton - '30, 19F and 31P. FT NMR, advantages of FT NMR, use of NMR in medicaldiagnostics.	e (*	
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#### Unit-III (A) Electron Spin Resonance Spectroscopy

Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the '9' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship, measurement techniques, applications.

#### (B) Nuclear Quadrupole Resonance Spectroscopy

Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splittings. Applications.

#### **Unit-IV X-ray Diffraction**

18Hrs

Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity'and electron density, phase problem. Description of the procedure for an X-ray structure analysis, absolute configuration of molecules, Ramchandran diagram.

#### **Books Suggested**

1. Modern Spectroscopy, J.M. Hollas, John Wiley.

- 2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and FL. Ho, Wiley Interscience.
- 3. NMR, NOR, EPB and Mossbauer Spectroscopy in Inorganic Chemistry, RV. Parish, Ellis Harwood.
- 4. Physical' Methods in Chemistry, FLS. Drago, Saunders College.
- 5. Chemical Applications of Group Theory, F. A. Cotton.
- 6. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
- 7. Basic Principles of Spectroscopy, Ft. Chang, McGraw Hill.
- 8. Theory and Applications of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH-Oxford.
- 9. Introduction to Photoelectron Spectroscopy, P. K. Ghosh, John Wiley.
- 10. Introduction to Magnetic Resonance, A Carrington and AD. Maclachalan, Harper & Row.

### CURRICULUM HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester - II Course CHNN- 505 (A)(Elective course) Organ transition Metal Chemistry Unit-I (A) Alkyls and Aryls of Transition Metals

**3Hrs** Types, routes of synthesis, stability and decomposition pathways, organocopper in organic Synthesis (B) Fluxional Organometallic Compounds 6Hrs Fluxionality and dynamic equilibria in compounds such as 112- olefin, n3~ allyl and dienyl complexes Unit-II (A) Compounds of Transition Metal-Carbon Multiple Bonds 9Hrs Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrOphilic reactions on the ligands, role in organic synthesis (B) Transition Metal Compounds with Bonds to Hydrogen 2Hrs Transition metal compounds with bonds to hydrogen. Unit-III Homogeneous Catalysis 10 Hrs Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (OXO reaction), oxopalladation reactions, activation of 0-H bond.

#### **Books Suggested**

- 1. Principles and Application of Organotransition Meta! Chemistry, J.P. Collman, L.S. Hegsdus, J.Fl. Norton and FLG. Finke, University Science Books. 2. The Organometallic Chemistry of the Transition Metals, RH. Crabtree, John Wiley
- 3. Metallo-organic Chemistry, A.J. Pearson, Wiley.
- 4. Organometallic Chemistry, RC. Mehrotra and A. Singh, New Age Internationa

### CURRICULUM

## HEMCHANDRACHARYA NORTH GUJARAT UNIVERSITY, PATAN M.Sc. (Chemistry) Semester – II Course CHNN – 505 (B)(Elective course) Bioinorganic and Supramolecular Chemistry

Unit-I (A) Metal Storage Transport and Biomineralization	3 Hrs
Ferritin, transferrin, and siderophores	
(B) Calcium in Biology	3 Hrs
Calcium in living cells, transport and regulation, molecular aspects of intramolecular	
processes, extracellular binding proteins	
Unit-II Metalloenzymes	12Hrs
Zinc enzymes carboxypeptidase and carbonic anhydrase. Iron enzymes catalase,	
peroxidase and cytochrome P-450. Copper enzymes superoxide dismutase.	
Molybdenum oxatransferase enzymes - xanthine oxidase. Coenzyme vitamin 812	
Unit-III Supramolecular Chemistry	12Hrs
Concepts and language.	
(A) Molecular recognition: Molecular receptors for different types of molecules including	
arisonic substrates, design and synthesis of coreceptor molecules and multiple	
recognition.	
(B) Supramolecular reactivity and catalysis.	
(C) Transport processes and carrier design.	
(D) Supramolecular devices. Supramolecular photochemistry, supramolecular electronic,	
ionic and switching devices.	R
Some example of self-assembly in supramolecular chemistry.	

### **Books Suggested**

- Principles of Bioinorganic Chemistry, 3.]. Lippard and J.M. Berg, University Science Books.
   Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
- 3. Inorganic Biochemistry vols I and II. ed. G.L. Eichhorn, Elsevier.
- 4. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley.
- 5. Supramolecular Chemistry, J.M. Lehn, VCH

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#### M.Sc. SEM - II

#### Practical I

### CHNN - 506 (Inorganic + Organic)

### Qualitative and Quantitative Analysis

A. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving

volumetric and gravimetric methods

#### Chromatography

Separation of cations and anions by

Paper Chromatography

Column Chromatography - Ion exchange.

#### Preparations

Preparation of selected inorganic compounds and their studies by I.R., electronic spectra,

Mossbauer, E.S.R. and magnetic susceptibility measurements. Handling of air and moisture

sensitive compounds.

- 1. VO(acac)2
- 2. TiO(C<sub>9</sub>H<sub>8</sub>NO)<sub>2</sub>2H<sub>2</sub>O
- 3. cis-K[Cr(C<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]
- 4. Na[Cr(NH<sub>3</sub>)<sub>2</sub>(SCN)<sub>4</sub>]
- 5. Mn(acac)3
- 6. K<sub>3</sub>[Fe(C<sub>2</sub>O<sub>4</sub>)3I
- 7. Prussian Blue, Turnbull's Blue.
- 8. Co(NH<sub>3</sub>)<sub>6</sub>] [CO(NO<sub>2</sub>)<sub>6</sub>]
- 9. cis-[Co(trien) (NO<sub>2</sub>)<sub>2</sub>]CI.H<sub>2</sub>O
- 10. Hg[Co(SCN)4]
- 11. [Co (Py)<sub>2</sub>Cl<sub>2</sub>]
- 12. [Ni (NH<sub>3</sub>)<sub>6</sub>]CI<sub>2</sub>
- 13. Ni(dmg)2
- 14. [Cu(NH<sub>3</sub>)<sub>4</sub>]SO<sub>4</sub>.H<sub>2</sub>0



#### **Books Suggested**

- 1. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS
- 2. Synthesis and Characterization of inorganic Compounds, W. L. Jolly, Prentice Hall
- 3. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller, Prentice Hall
- 4. Macroscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath.
- 5. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold.
- 6. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.

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- 7. Vogel's Textbook of Practical Organic Chemistry, A. Ft. Tatchell, John Wiley
- 8. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman
- 9. Findley's Practical Physical Chemistry, B. P. Levitt, Longman

10. Experimental Physical Chemistry, RC. Das and B. Behera, Tata McGraw Hill.

#### **Qualitative Analysis**



Separation, purification and identification of compounds of three component mixture

using tlc and column chromatography, chemical tests. IR spectra to be used for functional

group identification.

1) All solid

2) All liquid

3) Solid (S) + liquid (S)

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- 3. Experiments and Techniques in Organic Chemistry, D. Pasto, C. Johnson and M. Miller,
- 4. Macróscale and Microscale Organic Experiments, K. L. Williamson, D. C. Heath. 5. Systematic Qualitative Organic Analysis, H. Middleton, Adward Arnold. 6. Handbook of Organic Analysis- Qualitative and Quantitative, H. Clark, Adward Arnold.

- 8. Practical Physical Chemistry, A. M. James and F. E. Prichard, Longman
- Findley's Practical Physical Chemistry, B. P. Levitt, Longman
- 7. Vogel's Textbook of Practical Organic Chemistry, A. Ft. Tatchell, John Wiley 9. ringley's riactical rugarear vacuus y, B. r. Levitt, Longman 10. Experimental Physical Chenistry, RC. Das and B. Behera, Tata McGraw Hill.



MSc. SEM - II

Practical - II

### CHNN - 507 Physical Chemistry

### **Chemical Kinetics**

(i) Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.

(ii) Flowing clock reactions (Ref: Experiments in Physical Chemistry by Showmaker)

(iii) Determination of the primary salt effect on the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidised by persulphate ion) (vi) Oscillatory reaction.

### Solutions

(i) Determination of molecular weight of non-volatile and non-e/ectrolyte/electrolyte by cryoscome method and to determine the activity coefficient of an electrolyte. (ii) Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behaviour that occurs with a strong electrolyte.

Electrochemistry

(A) Conductometry

(i)To study the effect of solvent on the conductance of AgN03 etic acid and to determine the degree of dissociation and equilibrium constant in different vents and in their mixtures (DMSO; DMF, dioxane, acetone, water) and to test validity of Debye-Huckel-Onsager theory. (ii) Determination of the activity coefficient of zinc ions in thution of 0.002 M zinc sulphate

using Debye Hitckel's limiting law.

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### (B) Potentiometry/pH metry

I) Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.

II) Determination of temperature dependence of EMF of a cell.

III) Determination of the formation constant of silver-ammonia complex and stoichiometry of

the complex potentiometrically.

IV) Acid—base titration in a non-aqueous media using a pH meter.

V) Determination of activity and activity coefficient of electrolytes.

VI) Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.

VII) Determination of the dissociation constant of monobasic/dibasic acid by Albert-Serjeant method.

VIII) Determination of thermodynamic constants, AG, AS and AH for the reaction by e.m.f. method.

 $Zn + H_2SO_4 \longrightarrow ZnSO_4 + 2H$ 

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- 2. Synthesis and Characterization of inorganic Compounds, W. L. Jolly, Prentice Hall
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