

**Name of Institute: Indus Institute of Sciences, Humanities & Liberal Studies (IISHLS)**

**Name of Faculty: Dr. Paras Patel**

**Course code: MCH0321**

**Course name: Qualitative Spectroscopic Techniques**

Pre-requisites: B.Sc. Chemistry

Credit points:

L	T	P	C
4	0	0	4

Offered Semester: III – Analytical Chemistry

**Course Coordinator (weeks XX - XX)**

Full name: **Dr. Kuldeep Joshi**

Department with siting location: Chemistry Department

2<sup>nd</sup> Floor , Chemistry Lab-II

Telephone: EXT: 3213

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Consultation times: Friday (02:25 – 04:15)

**Course Lecturer (weeks xx - XX)**

Full name: **Dr. Paras Patel**

Department with siting location: Chemistry Department

B-424 , 4<sup>th</sup> Floor, Bhanwar Building

Telephone: EXT : 3404

Email: [paraspatel.gd@indusuni.ac.in](mailto:paraspatel.gd@indusuni.ac.in)

Consultation times: Friday, 03:30 PM – 05:00 PM)

Students will be contacted throughout the Session via Mail with important information relating to this Course.

## Course Objectives

By participating in and understanding all facets of this Course a student will:

## Course Outcomes (CO)

**CO 1:** Explain the theoretical foundation of the most commonly used spectroscopic techniques. [BT-2]

**CO 2:** Evaluate the chemical structure using NMR spectrum. [BT-5]

**CO 3:** Describe the Infrared and Raman spectroscopy with dipole moments. [BT-2]

**CO 4:** Discuss the principles of Mass spectrometry. [BT-2]

**CO 5:** Analyse the Mass spectra to evaluate the chemical structure. [BT-4]

**CO 6:** Summarize ESR, Mossbauer spectroscopy and its applications. [BT-2]

## Course Outline

(Key in topics to be dealt)

- Spectroscopic Techniques
- NMR
- Mass Spectroscopy
- Infrared Spectroscopy
- Raman Spectroscopy
- ESR
- Mossbauer Spectroscopy

## Method of delivery

(Face to face lectures, Active Learning Techniques)

## Study time

(04 Hours per week)

## CO-PO Mapping (PO: Program Outcomes)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10	PO 11	PO 12
<b>CO1</b>	2	2	-	1	1	-	-	-	-	-	-	-
<b>CO2</b>	3	1	-	1	-	2	-	-	-	-	-	-
<b>CO3</b>	2	-	2	2	-	2	3	-	-	-	-	-
<b>CO4</b>	1	1	-	1	-	-	-	1	-	-	-	-
<b>CO5</b>	1	3	1	2	-	-	-	-	1	-	-	-
<b>CO6</b>	2	2	-	1	-	-	-	-	2	-	-	-

## Blooms Taxonomy and Knowledge retention (For reference)

(Blooms taxonomy has been given for reference)

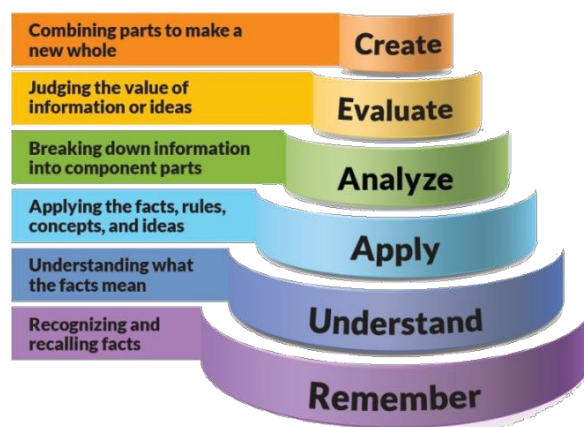


Figure 1: Blooms Taxonomy

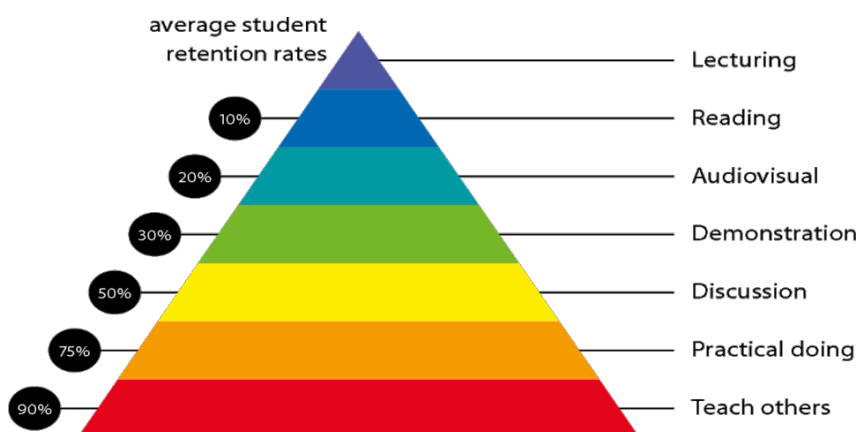


Figure 2: Knowledge retention

## Graduate Qualities and Capabilities covered

(Qualities graduates harness crediting this Course)

General Graduate Qualities	Specific Department of Chemistry Graduate Capabilities
<p><b>Informed</b></p> <p>Have a sound knowledge of an area of study or profession and understand its current issues, locally and internationally. Know how to apply this knowledge. Understand how an area of study has developed and how it relates to other areas.</p>	<p><b>1 Professional knowledge, grounding &amp; awareness:</b> - Student's will gain knowledge about chemistry subject in the both areas i.e. theory as well as practical's. Professionally students will know how chemistry is important in our daily life as well as to build up any industry. Students will be having knowledge/awareness about chemicals' such as how to use them and how hazardous they are for the environment.</p>
<p><b>Independent learners</b></p> <p>Engage with new ideas and ways of thinking and critically analyze issues. Seek to extend knowledge through ongoing research, enquiry and reflection. Find and evaluate information, using a variety of sources and technologies. Acknowledge the work and ideas of others.</p>	<p><b>2 Information literacy, gathering &amp; processing:</b> - Student's will be able identify the problems happening in the society as well as in the industry such as water quality, loss due to corrosion, pollutant coming from cement plant etc. with this basic information they will be having ability to gather the possible solutions.</p>

<p><b>Problem solvers</b></p> <p>Take on challenges and opportunities. Apply creative, logical and critical thinking skills to respond effectively. Make and implement decisions. Be flexible, thorough, innovative and aim for high standards.</p>	<p><b>3 Problem solving skills:</b></p> <p>Chemistry education provides students with the tools to solve problems. This means that students should be able to apply the scientific method: define a problem clearly, develop testable hypotheses, design and execute experiments, analyze data using appropriate statistical methods, and draw appropriate conclusions.</p> <p>Students should be able to integrate knowledge across chemical sub disciplines and apply this knowledge to solve problems. In the laboratory, in addition to the characteristics described above, students should understand the fundamental uncertainties in experimental measurements.</p>
<p><b>Effective communicators</b></p> <p>Articulate ideas and convey them effectively using a range of media. Work collaboratively and engage with people in different settings. Recognize how culture can shape communication.</p>	<p><b>4 Written communication: -</b></p> <p>Students should be able to retrieve specific information from the chemical literature, critically evaluate technical articles, and manage many types of chemical information. Students should develop proficiency with electronic searching of appropriate technical databases, including structure-based searching.</p> <p><b>5 Oral communication: -</b> Students should orally be able to use communication technology such as computerized presentations as well as software for word</p>
	<p>processing, chemical-structure drawing, and poster preparation and research paper presentation to any conferences.</p>

	<p><b>6 Teamwork:</b> - Students should be able to Solve scientific problems often involves working in disciplinary and multidisciplinary teams. This is especially true in industry and increasingly in academic settings. Students should learn to work productively with a diverse group of peers in classroom and laboratory activities. Students should be able to lead portions of an activity or be effective followers, as dictated by the situation. Peer- and self-assessment is often an effective way to evaluate student contributions to group activities.</p>
<p><b>Responsible</b></p> <p>Understand how decisions can affect others and make ethically informed choices. Appreciate and respect diversity. Act with integrity as part of local, national, global and professional communities.</p>	<p><b>7 Sustainability, societal &amp; environmental impact:</b> With this course students will know/ aware/ learn about the sustainable use of green products, proper management of renewable energy resources, and to find out new energy replacement sources. Students will be socially aware about the sources of pollutant that damages the water, soil, air etc. So they will be having capabilities/ knowledge how to tackled/ deal with different types of pollutions.</p>

### Practical work: NA

### Lecture/tutorial times

(Give lecture times in the format below)\_

*Example:*

*Lecture :*

*Lab :*

### Attendance Requirements

The University norms states that it is the responsibility of student s to attend all lectures, tutorials, seminars and practical work as stipulated in the Course outline. Minimum attendance requirement as per university norms is compulsory for being eligible for mid and end semester examinations.

## Details of referencing system to be used in written work

### Text books

1. Handbook of Instrumental Techniques for Analytical Chemistry, Frank Settle, Prentice Hall PTR, New Jersey, 1997.
2. Applied Infrared Spectroscopy, Smith A L, Wiley, New York, 1979.
3. Instrumental Methods of Analysis, Willard H H, 7th edition, Belmont, CA: Wadsworth, 1987.
4. Organic Spectroscopy, William Kemp, 3<sup>rd</sup> Edition, Palgrave Macmillan, 2008.
5. Raman Spectroscopy, Long D A, McGraw – Hill, New York, 1977.
6. Laboratory Raman Spectroscopy, Strommen D P, Nakamoto N, Wiley, New York, 1984.
7. Spectrometric Identification of Organic Compounds, Silverstein R M, Bassler G C, Morrill T C, 8th edition, Wiley, New York, 2015.
8. Introduction to NMR Spectroscopy, Abraham R J, Fisher J, Loftus P, Wiley, New York, 1988.
9. Elements of X – Ray Crystallography, Azaroff L V, McGraw – Hill, New York, 1998.
10. X–Ray Structure Determination: A Practical Guide, Stout G H, Jensen L H, 2nd edition, Wiley, New York, 1989

### Additional Materials

## ASSESSMENT GUIDELINES

Your final course mark will be calculated from the following:

❖ **Theory**

❖ CIE\_(60 marks)

1. Mid Semester Examination = 40 marks

2. Internal Evaluation = 20 marks

(Attendance = 5 Marks

Presentation =5 Marks

Assignment-I = 5 Marks

Assignment-II = 5 Marks

Total = 60 marks

❖ ESE\_(40 marks)

## SUPPLEMENTARY ASSESSMENT

Students who receive an overall mark less than 40% in mid semester or end semester will be considered for supplementary assessment in the respective components (i.e mid semester or end semester) of semester concerned. Students must make themselves available during the supplementary examination period to take up the respective components (mid semester or end semester) and need to obtain the required minimum 40% marks to clear the concerned components.

### Practical Work Report/Laboratory Report:

A report on the practical work is due the subsequent week after completion of the class by each group.

### Late Work

Late assignments will not be accepted without supporting documentation. Late submission of the reports will result in a deduction of -% of the maximum mark per calendar day



## Format

All assignments must be presented in a neat, legible format with all information sources correctly referenced. **Assignment material handed in throughout the session that is not neat and legible will not be marked and will be returned to the student.**

## Retention of Written Work

Written assessment work will be retained by the Course coordinator/lecturer for two weeks after marking to be collected by the students.

## University and Faculty Policies

Students should make themselves aware of the University and/or Faculty Policies regarding plagiarism, special consideration, supplementary examinations and other educational issues and student matters.

**Plagiarism** - Plagiarism is not acceptable and may result in the imposition of severe penalties. Plagiarism is the use of another person's work, or idea, as if it is his or her own - if you have any doubts at all on what constitutes plagiarism, please consult your Course coordinator or lecturer. Plagiarism will be penalized severely.

***Do not copy the work of other students.***

***Do not share your work with other students (except where required for a group activity or assessment)***

## Course schedule (subject to change)

(Mention quiz, assignment submission, breaks etc as well in the table under the Teaching Learning Activity Column)

Week #	Topic & contents	CO Addressed	Teaching Learning Activity (TLA)
Weeks 1	<b>Unit-I Nuclear Magnetic Resonance Spectroscopy (<math>^1\text{H-NMR}</math>):</b> Chemical and magnetic equivalent protons, Chemical shift, Spin-spin coupling	4	Chalk and Talk
Weeks 2	Different types of coupling, Factors affecting to coupling constant, Karplus equation, Spin system (AB, AX, ABX, AMX), Shift reagents, Nuclear Over Houser Effect (NOE).	4	Chalk and Talk
Week 3	<b>Nuclear Magnetic Resonance Spectroscopy (<math>^{13}\text{C NMR}</math>):</b> Introduction, Chemical shift of aliphatic, olefinic, alkyne, aromatic	4	Chalk and Talk
Week 4	heteroaromatic and carbonyl carbon, Effect of substituents on chemical shift	5	Chalk and Talk
Week 5	<b>Unit-II Mass Spectrometry:</b> Basic principles and brief outline of instrumentation, ion formation and types: relative abundances of isotopes and their contribution to characteristic peaks, mass spectrum; its characteristics, presentation and interpretation	5	Chalk and Talk

Week 6	chemical ionization mass spectrometry. Nitrogen rule, Mac-Lafferty rearrangement, Retro-Diels-Alder reaction.	1	Chalk and Talk
Week 7	<b>Ion sources-</b> matrix assisted laser desorption ionization (MALDI), thermospray, electrospray, atmospheric pressure chemical ionization (APCI),	1	Chalk and Talk
Week 8	atmospheric pressure photo ionization (APPI) and atmospheric pressure secondary ion ionization (APSI); Mass analyzers- quadrupole, ion-trap, time of flight (TOF), ion-cyclotron resonance and Fourier transform mass spectrometry.	1,6	Chalk and Talk
Week 9	<b>Unit-III Infra-Red Spectroscopy:</b> Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds),	1	Chalk and Talk
Week 10	Effect of hydrogen bonding, Solvent effect on vibrational frequencies, Overtones and Combination bands, Joint examples (UV, IR, NMR, Mass)	2	Chalk and Talk
Week 11	<b>Raman Spectroscopy:</b> Classical and Quantum theory of Raman Scattering, Experimental Methods, Correlation of Infrared and Raman Spectra, Normal Modes of vibrations.	2,6	Chalk and Talk Planned Test-2
Week 12	<b>Unit-IV</b> Molecular Spectroscopy: Optical transitions in molecules:	2	Chalk and Talk
Week 13	Rotational spectra, Vibrational spectra, Electronic Transitions,	2	Chalk and Talk
Week 14	Franck-Condon Principle. Principle, Instrumentation,	3	Chalk and Talk
Week 15	Applications of Electron Spin Resonance Spectroscopy (ESR), Mossbauer's Spectroscopy.	3	Chalk and Talk

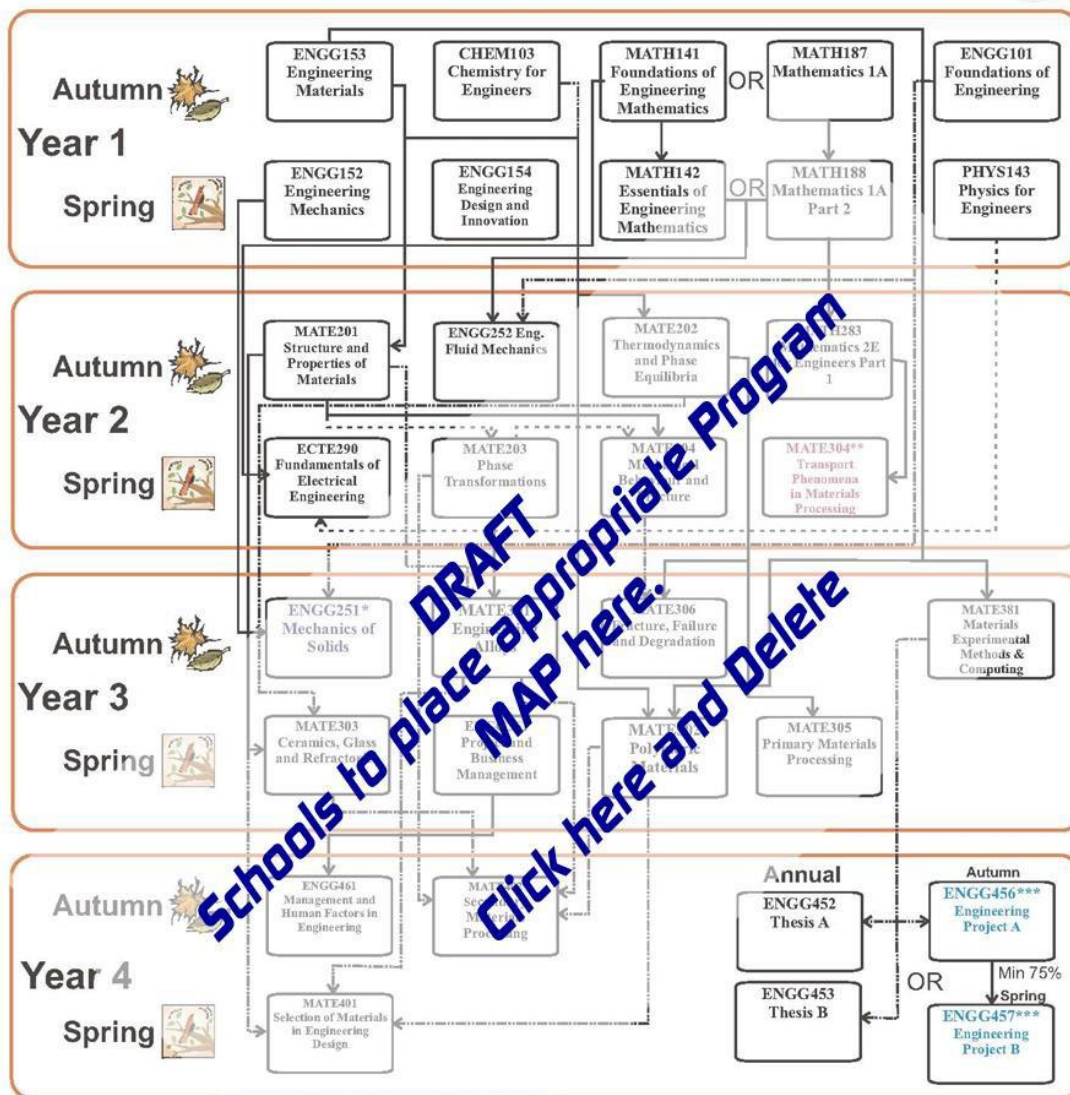
	Week 16	Submission and Viva	3	



# PROGRAM MAP for Bachelor of Engineering (Materials Engineering)



DEGREE - 2012



## Electives \*

MATE 411  
Advanced  
Materials  
and Processing

MATE412  
Electronic  
Materials

MATE413  
Structural  
Characterisation  
Techniques

MATE422  
Iron and  
Steelmaking

MATE433  
Surface  
Engineering

\* Note: Students will take three electives  
Some electives are only offered every 2nd year

ENGG251\* Note: Full time students entering Year 3 in 2012 will need to take one elective in Autumn as they have already completed ENGG251

MATE304\*\* Note: Full time students entering Year 3 in 2012 will need to take MATE304 in Spring of their 4th year or take it in 2012 and defer another subject to Spring 2012

ENGG456\*\*\*Note: If ENGG456 Engineering Project A (6cp) is done instead of a thesis, a student needs to complete 4 electives and is not eligible for honours

