Name of Institute: Indus Institute of Sciences, Humanities & Liberal Studies
Name of Faculty: Dr. Chetana Deoghare

Course code: MCH0303
Course name: Organic Spectroscopy
Pre-requisites: B. Sc. Chemistry

Credit points:

L	T	P	C
4	0	0	4

Offered Semester: III

Course Coordinator (week's XX - XX)
Full Name: Dr. Chetana Deoghare
Department with sitting location: Science and Humanities Department, 4th Floor, Bhanvar Building, Class Room No. 11.
Telephone: EXT: 3414
Email: chetanadeoghare.gd@indusuni.ac.in
Consultation times: Friday 3.20 pm to 4.15 pm

Course Lecturer (week's xx - XX)
Full name: Dr. Chetana Deoghare
Department with sitting location: Science and Humanities Department, 4th Floor, Bhanvar Building, Class Room No. 11.

Telephone: EXT: 3414
Email: chetanadeoghare.gd@indusuni.ac.in
Consultation times: Friday 3.20 pm to 4.15 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:

1. To study the working principles of Nuclear Magnetic Resonance Spectroscopy.
2. To study the working principles of C^{13} NMR and Mass Spectroscopy.
3. To study the working principles of and Infra Red Spectroscopy.
4. To study the working principles of Electron paramagnetic resonance Spectroscopy.
5. To analyze the structure of organic compounds using spectral data.

6. To explain the structural analysis of unknown organic compound.

Course Outcomes (CO)

After the successful completion of the course, students will be able to;

1) Identify organic compounds by analysis and interpretation of spectral data [BT1].
2) Explain common terms in NMR spectroscopy such as chemical shift, coupling constant, and anisotropy [BT2].
3) Analyse and interpret 1D and 2D NMR spectra of various organic compounds [BT4].
4) Describe the working principles of basic instruments used in organic analysis [BT2].
5) Calculate the mass unknown organic compounds using mass spectroscopy [BT3].
6) Solve chemical structural problems of organic compounds in a systematic manner using spectroscopy tools [BT3].

Course Outline

(Key in topics to be dealt)

- **Nuclear Magnetic Resonance Spectroscopy**
- **C^{13} NMR spectroscopy**
- **Mass Spectroscopy**
- **Infra Red Spectroscopy**
- **Electron paramagnetic resonance Spectroscopy**
- **Problems based on joint application**

Method of delivery

(Face to Face lectures, Active Learning Techniques, Power Point Presentations)

Study time

(How many hours per week including class attendance)

CO-PO Mapping (PO: Program Outcomes)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO10	PO11	PO12
CO 1	-	-	-	-	-	-	-	-	-	-	-	-

CO 2	-	-	-	-	-	-	-	-	-	-	-	-
CO 3	-	-	-	-	-	-	-	-	-	-	-	-
CO 4	-	-	-	-	-	-	-	-	-	-	-	-
CO 5	-	-	-	-	-	-	-	-	-	-	-	-
CO 6												

Blooms Taxonomy and Knowledge retention (For reference)

(Blooms taxonomy has been given for reference)

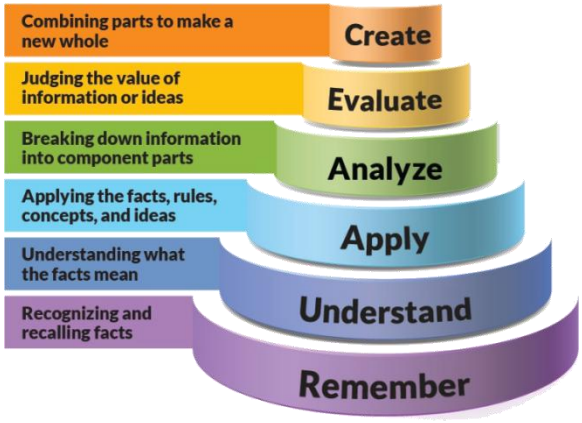


Figure 1: Blooms Taxonomy

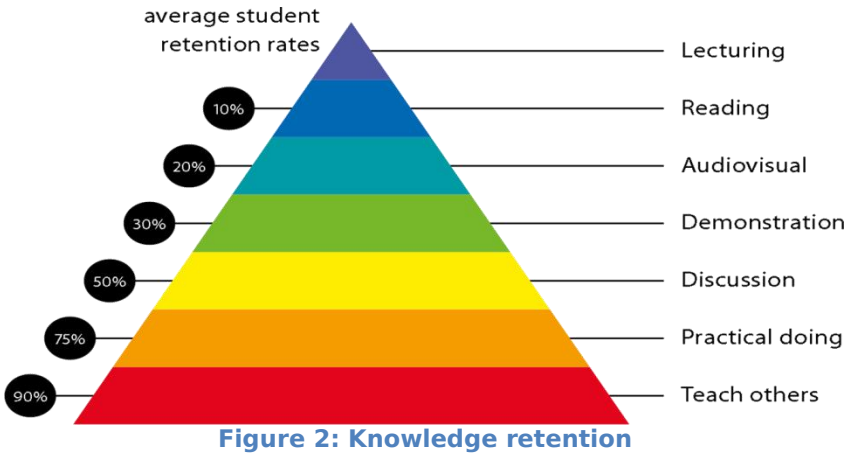


Figure 2: Knowledge retention

Graduate Qualities and Capabilities covered

(Qualities graduates harness crediting this Course)

General Graduate Qualities	Department of Chemistry Post Graduate Capabilities

Informed 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.	**1 Professional knowledge, grounding & awareness:-** 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.
Independent learners Engage with new ideas and ways of thinking and critically analyse 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.	**2 Information literacy, gathering & processing:-** Student's will be able identify the problems happening in the society as well as in the industry such as Photochemistry, uses of Aromatic heterocyclic compounds and their reactions, Organic waste coming from the industries etc. with this basic information they will be having ability to gather the possible solutions.
Problem solvers 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.	**4 Problem solving skills:** Organic Chemistry education provides students with the tools to solve many problems based on Chemistry. This means that students should be able to apply the scientific method: define a problem clearly, develop testable hypotheses, design and execute experiments, analyse data using appropriate statistical methods, and draw appropriate conclusions. 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.

Effective communicators 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.	**5 Written communication:-** 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 able to develop proficiency with electronic searching of appropriate technical databases, including structure-based searching.
	6 Oral communication:- Students should orally able to use communication technology such as computerized presentations as well as software for word processing, chemical-structure drawing, writing review article on any related topic, poster preparation and research paper presentation to any conferences.
	7 Teamwork:- 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.

Responsible 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.	**10 Sustainability, societal & environmental impact:** With this course students will know/ aware/ learn about the sustainable use of the organic reagents while performing the laboratory experiments. Students will be able to understand various photochemical reactions happening in the environment and their participation in global warming. So they will be having capabilities/ knowledge how to tackled/ deal with different types of organic pollutants coming from the organic laboratory and industry.

Practical work: NA

(Mention what practical work this Course involves)

Lecture/tutorial times

(Give lecture times in the format below)

Attendance Requirements

The University norms states that it is the responsibility of students 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

1. Introduction to spectroscopy, D. L. Pavia, G. M. Lampman, J. R. Vyvyan and G. S. Kriz, 3rd edition, Harcourt college publishers.
2. Spectrometric identification of organic compounds, T. C. Morril R. M. Silverstein and G. Bassler, 6th edition, John Wiley and sons.
3. Spectroscopic methods in organic chemistry, D. H. Williams and Tanfleming.

4. C. N. Banwell, Fundamentals of molecular Spectroscopy, 3rd ed., TMH, New Delhi, 1983. 5.
5. B. P., Straughan and S. Walker, Spectroscopy, Vol.3, Chapman Hall, London, 1976.
6. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1964.

Text books

1. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley New York, 1989.
2. P. S. Kalsi, Spectroscopy of Organic Compounds, 6thEdition, New age international publishers, 2007.
3. Clegg, W., Crystal structure determination, Oxford University press, New York,1998.
4. Stout, G. H., Jensen, L.H. X-ray structure determination: A practical guide, John wiley & sons Publication: New York, 1989.
5. Glusker, J. P. Trueblood, K. N. Crystal structure analysis: A primer., Oxford university press, New York, 1972.

Additional Materials: NA

ASSESSMENT GUIDELINES

Your final course mark will be calculated from the following:

- **Theory**
- CIE (60 marks)
  1. Mid semester Examination = 40 marks
  2. Attendance = 5 marks
  3. Presentation = 5 marks
  4. Assignment = 10 marks

  Total = 60 marks

- ESE (40 marks)
  1. Theory Exam = **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)

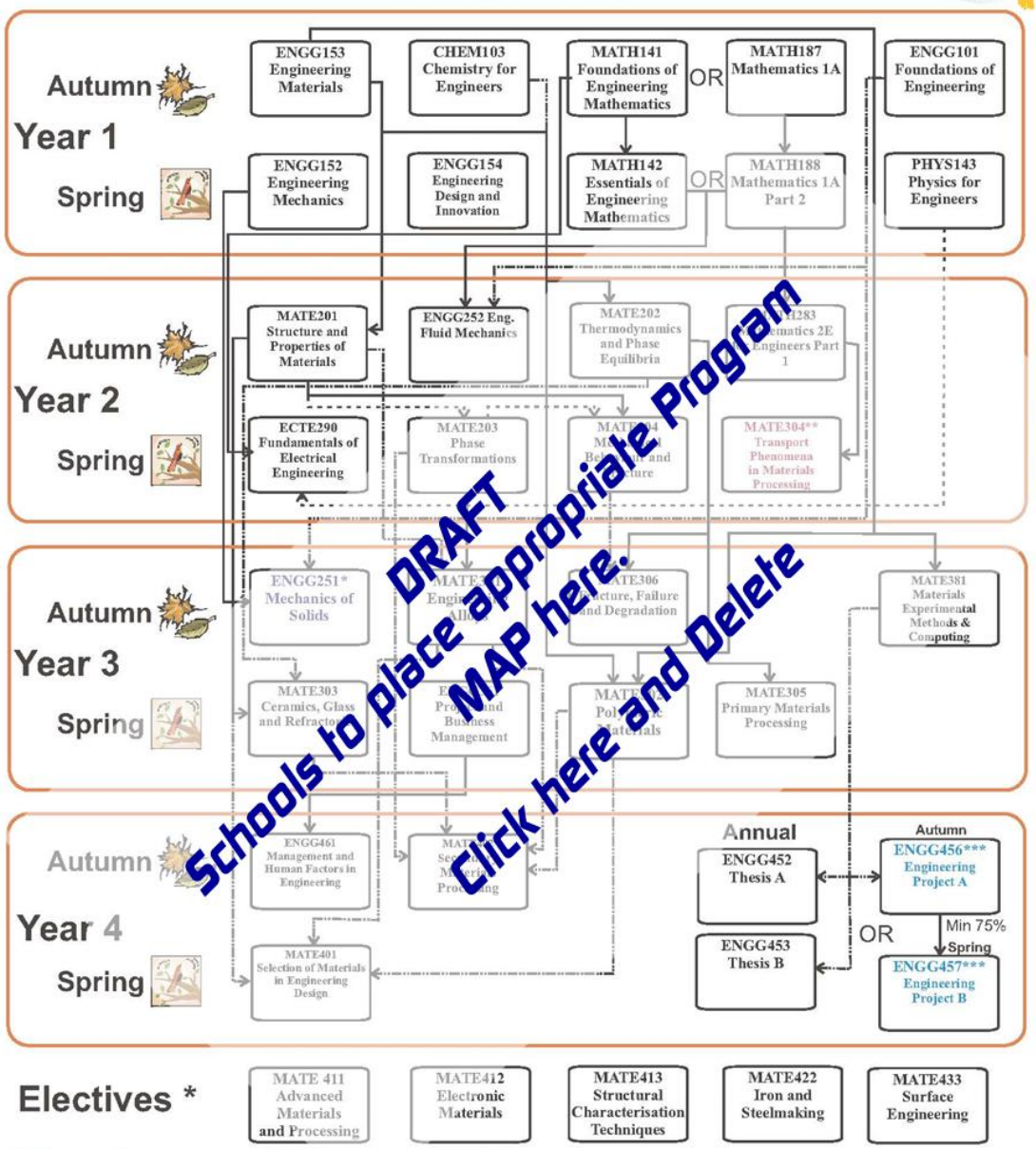
(Mention quiz, assignment submission, breaks etc as well in the table under the Teaching Learning Activity Column)

	Week #	Topic & contents	CO Addressed	Teaching Learning Activity (TLA)
	Weeks 1	**Nuclear Magnetic Resonance (NMR) Spectroscopy:** Elementary ideas of NMR integration, chemical shifts, Factors affecting, chemical shifts, coupling (first order, analysis) instrumentation and principles and instrumentation	1,2 &3	
	Weeks 2	FT, chemical shifts, spin-spin coupling different spin systems, mechanism of spin coupling. E.g. AB, ABX,	1,2 &3	
	Week 3	factors affecting vicinal and geminal couplings, rate processes, long range couplings, spin decoupling,	1,2 &3	
	Week 4	Shift reagents, solvent shifts, and nuclear overhauser effect. 2D NMR (COSY and HETCOR) applications.	1,2 &3	
	Week 5	**C^{13} NMR:** Elementary ideas, instrumental problems, chemical shift features of hydrocarbons,	1 & 5	
	Week 6	effect of substituent on chemical shifts olefinic, acetylenic, aromatic and carbonyl carbons, effects of coupling.	1 & 5	
	Week 7	**Mass spectrometry:** Theory, instrumentation, modes of ionization, types of detectors, modes of fragmentation.	1 & 5	
	Week 8	Different types of ions, molecular ions, isotopic peaks, factors controlling fragmentation, hyphenated mass spectroscopy techniques.	1 & 5	
	Week 9	**Detectors:** Quadrupole mass filter, time of flight (TOF). EI mass spectra interpretation: intensity of molecular ion peak,	1 & 5	Mid Semester Exam

		base peak, fragment ion peak and isotope peak (M+1), (M+2);		
	Week 10	Nitrogen rule, molecular formula determination (rule of 13), fragmentation pattern and McLafferty rearrangement, fragmentation of functional groups, hydrocarbons, ethers, aldehyde, ketone, acids, esters, amide, sulfur, and halogen compounds.	1 & 5	
	Week 11	**IR:** Vibrational transitions, important group frequencies	1 & 5	
	Week 12	factors affecting I.R. group frequency, applications of I.R. instrumentation.	3 & 5	
	Week 13	**Electron paramagnetic resonance (EPR) Spectroscopy:** Introduction, energy of transition and energy	1,3 &5	
	Week 14	levels, instrumentation, Zeeman effect, hyperfine interaction,	1,3 &5	
	Week 15	Structural elucidation of drug molecules based on joint application of UV, IR, ^{1}HNMR, ^{13}CNMR, EPR and mass spectroscopy.	1,3 &5	
	Week 16	Structural elucidation of drug molecules based on joint application of UV, IR, ^{1}HNMR, ^{13}CNMR, EPR and mass spectroscopy.	1,3&5	

PROGRAM MAP for Bachelor of Engineering (Materials Engineering)

DEGREE - 2012



* 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