

**NIZAM COLLEGE : DEPARTMENT OF CHEMISTRY**  
**LESSON PLAN FOR THE ACADEMIC YEAR 2018-2019 (Semester IX)**

**Class : FIVE YEAR INTEGRATED COURSE IN CHEMISTRY (FYIC) – V year**

**Paper-I FYIC 901 INORGANIC CHEMISTRY** (Bonding, Group Theory and its Applications)

IC-01: Group Theory, Normal mode analysis and Spectral Activity

S.No.	Topic	Hours
1	Properties of a point group, closure rule-abelion and non-abelion groups, associative rule, inverse rule and identity rule.	1
2	Group multiplication table, the rearrangement theorem, GMT of $C_3$ , $C_4$ , $C_{2v}$ , $C_{2h}$ , $C_{3v}$ and $C_5$ point groups	2
3	Sub groups-Langrange's theorem, Classes, similarity transformation. Properties of conjugate elements, definition, classes for $C_{2v}$ , $C_{3v}$	2
4	Matrices and vectors, types of matrices, multiplication and direct product, matrix representation of symmetry elements-E, $\sigma$ , $i$ , $C_n$ and $S_n$ .	2
5	Matrix representation of point groups, product and square rule, Matrices of $C_{2h}$ , $C_{2v}$ , $C_{3v}$ and $C_{4v}$ , block factorization	1
6	Transformation matrices, reducible and irreducible representations, character of a representation, properties of irreducible representation, orthogonality principle, construction of character table	2
7	Character tables of $C_{2h}$ , $C_{2v}$ , $C_{3v}$ and $C_{4v}$ groups	1
8	Mulliken symbolism, rules for IRs. Symmetry species for translations and rotations, standard reduction formula	1
9	The direct product, rules of direct products, normal mode analysis, Cartesian coordinate method, $C_{2v}$ , alternate method	1
10	Internal coordinate method $C_{2v}$ - $H_2O$ , IR and Raman activity	1
11	Normal mode/Internal coordinate method for $C_{2h}$ and $C_{3v}$ with examples	1

IC-02: MOT of Metal Complexes

S.No.	Topic	Hours
1	Limitations of CFT, Adjustments of CFT to allow for covalence	1
2	Experimental evidences for metal-ligand orbital overlap – ESR and NMR studies of few metal complexes	1
3	Adjusted CFT, introduction to MOT	1
4	Symmetry classification of metal and ligand orbitals in non-cubic environment, square pyramidal, trigonal bipyramidal and square planar geometries	2
5	Concept of LGO's, LCAO concepts	1
6	Construction of LGO's for $O_h$ , $T_d$ and $Sq$ pl geometries	1
7	Construction of MOED – $O_h$ metal complexes with $\sigma$ orbitals, $\sigma$ and $\pi$ orbitals, $\sigma$ , $\pi$ and $\pi^*$ orbitals	2
8	Construction of MOED for $T_d$ metal complexes with $\sigma$ and $\pi$ orbitals	1
9	Construction of MOED for square planar metal complexes with $\sigma$ and $\pi$ orbitals	2
10	MO electronic configuration and calculation of magnetic moment	

### IC-03: Electronic Spectroscopy of Metal Complexes

Topic to be covered	No. of hours
Introduction to crystal field diagrams-construction of CFELD of Oh, Td, Square planar geometries, construction of ligand field diagrams- effect of weak crystal field on S, P, D, f terms	1
Construction of Orgel diagrams- $d^1, d^6, d^9, d^4$ ; $d^2, d^7, d^8, d^3$ ; $d^5$ configurations, concept of hole formalism, expected electronic transitions	1
Construction of correlation diagram for $d^2$ Oh environments-strong field configurations-calculation of no. of microstates for each strong field configuration by direct product method, and method of descending symmetry. Rule of correspondence and non crossing rule	2
Correlation diagram for Td environment and other for other configurations discussion	1
Tanabe-Sugano Diagrams-construction for $d^2$ and $d^8$ configuration, comparison of Orgel and Tanabe-Sugano diagrams	2
Classification of electronic spectra –ligand field spectra and charge transfer spectra, types of electronic spectral recordings-solid, solution spectra.	1
Selection rules for electronic spectra-orbital selection rules-transitions between two non-degenerate states, transitions between states of different degeneracy, two electron transitions	1
Spin selection rules, relaxation in rules-departure from cubic symmetry, d-p mixing, vibronic coupling, magnetic dipole transitions	1
Nature of spectral bands- band intensities-intensity of d-d band, intensity of C-T band, band widths-variation in $10Dq$ , lower symmetry components	1
Franck-Condon principle, spin orbit coupling, Jahn-Teller effect,	1
Experimental evidence, dynamic JT effect	1
Spectrochemical series-factors affecting $10Dq$ , Nephelauxetic series	1
Examples of metal complexes and their detailed electronic spectral characterization with values	1
<b>Total</b>	<b>15</b>

### IC-04: IR and Raman Spectroscopy

Topic to be covered	No. of hours
Introduction to molecular spectra, nature of electromagnetic radiation, mechanism of interaction and Hooke's law, force constants, potential energy curve for a vibrating molecule	1
Selection rules-conditions for IR activity-HOMO nuclear diatomics and HETERONuclear diatomics, polyatoms	1
Anharmonicity of molecular vibrations and potential energy functions,	1
Fundamental bands, overtones, and hot bands, Fermi resonance	1
Partial normal mode analysis-finding out the molecular point group, character table and calculating the no. of reducible representations from standard reduction formula, classifying the RR's into vibrations, rotations and assignment of IRR's for the modes.	3
Few more examples for normal mode analysis	1
Determination of coordination sites and linkage isomers like $NO_2$ and $SCN$ , denticity of $SO_4^{2-}$ , $CO_3^{2-}$	1
Distinguishing geometrical isomers- cis & trans, fac and mer isomers	1
Effect of coordination on ligand vibrations-mono, bi, polydentate ligands of oxygen, nitrogen, carbon and halogens-NH, $H_2O$ , Glycine, Carbonyl and halides	1
Prediction of diagnostic fundamentals of geometrical isomers of metal complexes, distinguishing isomers of metal complexes	1
Discovery of Raman effect-Raman experiment, Raman lines-stokes, anti stokes, Rayleigh scattering, conditions for Raman activity-polarizability	1
Raman spectra of $CO$ , $HCN$ , $CO_2$ , $NO_2$ , $H_2O$ , principles of resonance Raman spectra	1
Structural elucidation of the active sites of Heme and non heme oxygen carriers.complementary nature of IR and Raman spectra.	1
<b>Total</b>	<b>15</b>

## Paper II FYIC 902 ORGANIC CHEMISTRY

OC- 01: New synthetic reactions

Topics to be covered	No. of Hours
<b>Metal mediated C-C and C-X coupling reactions:</b> Introduction to Metal mediated C-C and C-X coupling reactions; General Reaction mechanism of transition metal mediated C-C and C-X reactions	2
Suzuki Coupling Reaction; Heck Coupling Reaction; Stille Coupling Reaction	1
Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions	1
<b>C=C Formation Reactions:</b> Importance of double bonded compounds; Introduction toC=C Formation Reactions	1
Shapiro, Bamford-Stevens andMcMurrey reactions	1
Julia-Lythgoe olefination and Peterson's stereoselective olefination	1
<b>Multicomponent Reactions:</b> Importance of Multicomponet reactions; Ugi and Passerini reactions	1
Biginelli, Hantzsch and Mannich reactions	1
<b>Ring Formation Reactions:</b> Pausan-Khand reaction, Bergman cyclisation, Nazarov cyclisation	1
<b>Click Chemistry:</b> Overview of Click Reactions; Criteria for Click reaction	1
Sharpless azides cycloadditions	1
<b>Metathesis:</b> Grubb's 1st and 2nd generation catalyst; Olefin cross coupling metathesis(OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications	1
<b>Other important synthetic reactions:</b> Baylis-Hilman reaction and Eschenmoser-Tanabe fragmentation	1
Mitsunobu reaction, Stork-enamine reaction and Michael reactions	1
	<b>15hrs</b>

**Course/Paper: IV- FYIC 904 (ANALYTICAL TECHNIQUES, SPECTROSCOPY and GREEN CHEMISTRY)**

**Unit: GC-01: Atomic Spectroscopy**

**No. of Hours Allotted: 15**

<b>Topics to be covered</b>	<b>No. of Hours</b>
Atomic Absorption Spectroscopy - Principle of AAS, quantitative methodology	1
Instrumentation – flame AAS and furnace AAS, resonance line sources - hollow cathode lamp.	1
Atomisers, monochromators, detectors, readout devices.	1
Graphite furnace atomic absorption spectroscopy - advantages and disadvantages.	1
Single beam atomic absorption spectroscopy, double beam atomic absorption spectroscopy.	1
Sensitivity and detection limits in AAS	1
Interferences atomic absorption spectroscopy – chemical, spectral, physical interferences.	1
Evaluation methods in AAS and application in qualitative and quantitative analysis.	1
Atomic Emission Spectroscopy - Introduction, Principles of AES	1
Instrumentation - dc arc, ac spark, dc plasma, universal arc-spark	1
Interferences, evaluation methods, Application in quantitative analysis	1
<b>Inductively Coupled Plasma - Atomic Emission Spectroscopy (ICP-AES) -</b> Limitations of AES, introduction to ICP- AES, characteristics of plasma.	1
Principles of plasma spectroscopy, plasma as an excitation source.	1
Inductively coupled plasma source, ICP-AES – Instrumentation, sample introduction, , monochromators, dectectors, processing and readout.	1
Application of ICP-AES, Comparison with AAS	1
	<b>15hrs</b>

Name of the Teacher: **Kavitha Ramdas**

Head, Department of Chemistry

Topics to be covered	No. of Hours
Optical Rotatory Dispersion (ORD) and CD Spectroscopy Optical rotation, Plane polarised light & LCP, RCP	1
circular birefringence, circular dichroism.	1
Cotton effect, Plain curves and anomalous curves	1
Determination of configuration of cyclic systems by comparing with known steroidal skeletal system	2
the octant rule Empirical and semiempirical rules-The axial haloketone rule and examples	1
Helicity rule, Exciton chirality method. Application of the rules to the study of absolute configuration and conformations of organic molecules.	1
Principles of 2D NMR, Classification of 2D-experiments.	1
Correlation spectroscopy (COSY) different examples	1
HOMO COSY (1H-1H COSY) -Examples	1
TOCSY (Total Correlation Spectroscopy),	1
Hetero COSY (1H13C COSY,HMQC),	1
long range 1H,13C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy	1
NOESY and 2D-INADEQUATE experiments and their applications	2
	<b>15hrs</b>

Name of the Teacher: **Dr. P.Sarita Rajender**

Head, Department of Chemistry

Topics to be covered	No. of Hours
<b>X-Ray Diffraction Methods:</b> Introduction to diffraction phenomenon; X-rays-introduction to X-rays, their discovery, production – discharge tube, theory of generation of X-rays; instrumentation, detection methods – photographic and counter methods.	1
Bragg's equation, Miller indices – calculation of miller indices; Methods of Diffraction – powder and single crystal methods.	1
Laue's photographic method – description of the method and detection, Bragg's X-ray spectrometric method – instrumentation and detection of diffracted X-rays.	1
Bragg's method for deduction of crystal structures – fcc, bcc and simple cubic structures. Deduction of structures of NaCl and KCl.	1
Rotating crystal method – methodology and detection, Powder X-ray diffraction method-instrumentation, diffraction cones/rings, detection on comparison with standard spectra.	1
Indexing reflections, systematic absences, reciprocal lattice concepts; Diffraction studies – contour / electron density maps.	1
Electron density studies of platinum pthalocyanine complex – contour maps and assignment of the atoms on respective positions on contour maps.	1
Electron density studies on silyl acetate and tetra alkyl biphosphate.	1
Advantages of X-ray diffraction studies – determination of bond length, bond angle, no. of bonds; Limitations of XRD.	1
<b>Electron diffraction by Gases:</b> Electron diffraction - introduction, principle and instrumentation.	1
Radial distribution curves; Interpretations of results for PBrF <sub>2</sub> S, PF <sub>3</sub> HS, PF <sub>2</sub> HS.	1
Interpretation of results for HClO <sub>4</sub> , silyl monothioacetate and Germyl monothioacetate; HgCl <sub>2</sub> molecule. Advantages and limitations of electron diffraction studies.	1
<b>Neutron diffraction:</b> Principle, sources used for neutron diffraction – fast neutrons – their isolation	1
Applications of neutron diffraction in hydrogen bonding studies, combined use of XRD and Neutron diffraction studies; Advantages and limitations of neutron diffraction studies.	1
Discussion – XRD, Electron and neutron diffraction	1
	<b>15hrs</b>

Name of the Teacher: **Dr. A.V.Aparna**

Head, Department of Chemistry