ACADEMIC AFFAIRS OFFICE
INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

No. Acd./3163 /IAPC-78 Dated: February 05 , 2020

Head, Department of Chemistry
(through e-mail)

The IAPC in its 78th meeting held on 31.12.2019 vide **Item No. 78.3.1** approved the following Pre-Ph.D. courses of Department of Chemistry with minor revision **(Appendix-A)**:

1. **CYN-902: Advanced Inorganic Chemistry**
2. **CYN-903: Advanced Organic Chemistry**
3. **CYN-904: Advanced Physical Chemistry**
4. **CYN-905: Spectroscopic Methods of Structural Elucidation**

Assistant Registrar (Curriculum)

Encl: as above

Copy to (through e mail):-

1. All faculty
2. All Heads of Departments/ Centres
3. Dean, Academic Affairs
4. Associate Dean of Academic Affairs (Curriculum)
5. Channel I/ Academic webpage of iitr.ac.in

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: Department of Chemistry

1. **Subject Code:** CYN-902 **Course Title:** Advanced Inorganic Chemistry
2. **Contact Hours:** **L:** 3 **T:** 0 **P:** 0
3. **Examination Duration (Hrs.):** **Theory** 3 **Practical:** 0
4. **Relative Weightage:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 3 **6. Semester:** Both **7. Subject Area:** PEC
8. **Pre-requisite:** Nil
9. **Objective:** To familiarise the students with recent topics required for inorganic chemistry research

10. Details of Course:

S. No.	Contents	Contact Hours
1	**Applications of Group Theory in Inorganic Chemistry:** Spectroscopic term symbols for free ions, metal complexes in octahedral, tetrahedral, square planar, square pyramidal complexes; use of irreducible representations for translations, rotations and vibrations in these molecules and their theoretical interpretation for infra-red and Raman transitions.	**14**
2	**Current trends in Organometallic Chemistry:** Organometallic approach to water splitting, role of osmium, ruthenium, titanium, manganese complexes in water splitting, homolytic activation of water with nickel, closed circle water splitting model, E-H bond activation of ammonia and water by phosphorous compounds, oxygen atom transfer reactions, role of pincer ligands, multimetallic catalysis based on heterometallic complexes.	**14**
3	**Current trends in Bioinorganic Chemistry:** Biological and synthetic oxygen carrier, platinum anticancer drugs and interaction of cisplatin with glutathione in cancel cell, types of superoxide dismutases – their active site structure and reaction mechanism, dioxygen activation by iron and copper enzymes, biomineralization, scorpionate ligands and hybrid materials for metalloenzyme models.	**14**
	Total	**42**

11. Suggested books:

S. No.	Authors/Title/Publishers	Year of Publication/ Reprint
1	Cotton, F. A. "Chemical Application of Group Theory" Wiley Student Edition, 3rd ed.	**2008**
2	Crabtree, R. H., "Organometallics and Catalysis: An Introduction", Wiley, 6th ed.	**2014**
3	Hartwig, J. F., "Organotransition Metal Chemistry: From Bonding to Catalysis", University Science Books.	**2010**
4	Research papers on the above mentioned topics	**2019**

INDIAN INSTITUTE OF TECHNOLOGY ROORKEE

NAME OF DEPTT./CENTRE: Department of Chemistry

1. **Subject Code:** CYN-903 **Course Title:** Advanced Organic Chemistry
2. **Contact Hours:** **L:** 03 **T:** 0 **P:** 0
3. **Examination Duration (Hrs.):** **Theory:** 3 **Practical:** 0
4. **Relative Weightage:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 3 **6. Semester:** Both **7. Subject Area:** PEC
8. **Pre-requisite:** Nil
9. **Objective:** To familiarise the students with recent topics required for organic chemistry research

10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Art in organic synthesis**: General considerations (realistic mechanisms, HSAB concept, Curtin-Hammett principles, homogeneous or heterogeneous systems, thermodynamic allowance, linear vs convergent methods), oxidation level of carbon centers in functional groups, isohypsic and non-isohypsic reactions, synthetic equivalency of functional groups, design of chemoselective, regioselective and steroselective reactions, renewable feedstocks as synthons, umpolung in synthesis, synthesis of cyclic molecules, radical reactions for cyclisations (Coreys's □-lactone synthesis)	**8**
2.	**Side reactions in Organic Synthesis:** Stability of organic compounds, stability towards oxygen (H-abstraction, SET mechanism), strained bonds, incompatible functional groups, detonating compounds, nature of electrophiles in nucleophilic substitution, effects of heteroatoms in electrophiles (nitrogen, halogen, silicon, boron), allylic and propargylic electrophiles, acylation reaction with problematic amines and alcohols (sterically and electronically deactivated amines, aminoacids, base labile alcohols), β-hydride elimination, protodematalation, dimerization as major side reactions in transition metal catalyzed organic synthesis	**6**
3.	**Green chemistry in organic synthesis:** Principles of green chemistry, atom economy and scope, preparation of green matrix, alternatives to common organic synthetic methods, microwave assisted organic synthesis (equipment, activation benefit, limitations, microwave effects in synthesis, some exemplary synthesis under microwave irradiation), visible light photochemistry (fundamentals of photocatalysis, metal complexes and organic dyes as photocatalysts, visible light photocatalysis in C-H activation reactions, atom transfer radical addition reaction, difunstionalization of alkenes and alkynes, □-amino functionalization reactions), organic synthesis in water (basic requirements, in-water and on-water synthesis, formation of trans phase, exemplary methods), mechanochemistry (ball mills in organic synthesis, use of stress in cleaving bonds, exemplary methods), organocatalysis (Aldol reaction, acyl transfer reactions, Setter reaction, Baker's yeast, N-heterocyclic carbenes) Ionic liquids (introduction and application in organic synthesis).	**14**
4.	**Modern methods of heteroaromatic synthesis**: Systematic nomenclature of heterocyclic compounds (Hantzsch Widman, replacement and fusion methods), synthesis of heterocyclic compounds based on transition metal catalyzed chemistry	**14**

	using Cu, Pd, Co and Ni (transition-metal-catalysed carbene coupling reactions, tandem catalytic reactions, carbonylation of acyclic precursors, cycloisomerizations of allenes with amine, amide, or sulfonamide nucleophiles, incorporation of chemo-, regio-, and stereocontrol in heterocyclic synthesis), synthesis and reactivity of hypervalent iodine compounds, applications of hypervalent Iodine(III) reagents in the constructions of heterocyclic compounds through oxidative coupling reactions, multicomponent reactions, use of multicomponent reactions in heterocyclic synthesis, Biginelli condensation, Kabachnik−Fields reaction, van Leusen method, Ugi reaction, Passerini Reaction and their postcondensation modifications, Knoevenagel-induced domino reactions, synthesis of heterocycles in nature, applications of heterocycles in pharmaceuticals, materials and agrochemicals	
	Total	**42**

11. Suggested Books

S. No.	Name of Authors /Books/Publishers	Year of Publication/ Reprint
1.	Smit, W. A., Bochkov, A. F., Caple, R., "Organic Synthesis, The Science behind the Art", The Royal Society of Chemistry, London.	1998
2.	Dörwald, F. Z., "Side Reactions in Organic Synthesis, A Guide to Successful Synthesis Design", WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim	2005
3.	Lancaster, M., "Green Chemistry, an Introductory Text", The Royal Society of Chemistry, London.	2002
4.	Kotschy, A., Timári, G., "Heterocyles from Transition Metal Catalysis, Formation and Functionalization", Springer, The Netherlands.	2005
5	Orru, R. V. A., Ruijter, E. (Ed), "Synthesis of Heterocycles via Multicomponent Reactions I, Springer-Verlag, Berlin Heidelberg.	2010

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NAME OF DEPTT./CENTRE: Department of Chemistry

1. **Subject Code:** CYN-904 **Course Title:** Advanced Physical Chemistry
2. **Contact Hours:** **L:** 03 **T:** 0 **P:** 0
3. **Examination Duration (Hrs.):** **Theory:** 3 **Practical:** 0
4. **Relative Weightage:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 3 **6. Semester:** Both **7. Subject Area:** PEC
8. **Pre-requisite:** Nil
9. **Objective:** To familiarise the students with recent topics required for physical chemistry research

10. Details of the Course:

S. No.	Contents	Contact Hours
1.	**Quantum Mechanics:** Brief review of the postulates and various models, Hydrogen like and many electron systems, Slater determinants for ground and excited states of atoms. approximation methods, Hartree-Fock methods, Electron correlation and post Hartree-Fock methods.	7
2.	**Density Functional Theory:** Electron density and hole functions, The Hohenberg-Kohn theorems, the Kohn-Sham approach, exchange-correlation functionals	7
3.	**Statistical Thermodynamics:** The statistical method and ensembles, microcanonical ensemble, canonical ensemble, generalized ensembles, connection of ensemble formalisms to thermodynamics, Fermi-Dirac and Bose-Einstein statistics, phase space and Liouville equation, non-equilibrium statistical mechanics: affinities and fluxes, Onsager's regression hypothesis, time correlation functions, response functions.	14
4.	**Spectroscopy**: Phenomenological treatment of absorption, emission, and scattering. Einstein coefficients, spectral lineshapes, and Principles of laser emission. Time dependent perturbation theory, transition probabilities – Fermi Golden Rule, Finite lifetime of states. Rotational spectroscopy: fundamentals of rotational spectra of diatomic molecules and polyatomic molecules: spherical, symmetric, and asymmetric tops. Vibrational spectroscopy: vibration of diatomic molecules, harmonic and anharmonic oscillator, vibration of polyatomic molecules. Normal modes and group theory. Fermi interactions, vibrational angular momentum, Coriolis perturbations and inversion doubling. Electronic spectroscopy of molecules: electronic absorption spectra of diatomic molecules. Molecular orbitals and term symbols. Dissociation and pre-dissociation in the spectra of diatomic. Introduction to non-linear spectroscopy: two-photon and higher order processes and their applications	14
	Total	42

11. Suggested Books

S. No.	Name of Authors /Books/Publishers	Year of Publication/ Reprint
1.	Schatz, G. C., Ratner M. A. "Quantum mechanics in chemistry", Prentice Hall	2002
2.	Szabo, A., Ostlund, N. S., "Modern quantum chemistry", 1st Revised Edn, Dover Publishers.	2008
3	Cramer, C. J., "Essentials of computational chemistry", 2nd ed., John Wiley & Sons Ltd, West Sussex, England.	2002
4.	W. Koch, Holthausen, M. C., "A chemist's guide to density functional theory", 2nd ed., Wiley-VCH Verlag Gmbh, Weinheim, Germany	2001
5.	McQuarrie, D. A., "Statistical mechanics", 1st Ed., Viva Books.	2011
6.	Callen, H. B., "Thermodynamics and an introduction to thermostatistics", 2ed Ed, Wiley.	2006
7.	Chandler, D., "Introduction to modern statistical mechanics", Oxford University Press, Cambridge.	1987
8.	Bernath, P. F., "Spectra of atoms and molecules", Oxford University Press, Cambridge	2005
9.	Hollas, J. M., "Modern spectroscopy", Wiley.	2003
10.	Boyd, R. W., "Nonlinear optics", Academic Press	2009

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NAME OF DEPTT/CENTRE: CHEMISTRY

1. **Subject Code:** CYN-905 **Course Title:** Spectroscopic Methods of Structural Elucidation
2. **Contact Hours:** **L:** 3 **T:** 1 **P:** 0
3. **Examination Duration (Hrs.):** **Theory:** 3 **Practical:** 0
4. **Relative Weight:** **CWS:** 20-35 **PRS:** 0 **MTE:** 20-30 **ETE:** 40-50 **PRE:** 0
5. **Credits:** 4 **6. Semester:** Both **7. Subject Area:** PEC
8. **Pre-requisite:** Nil
9. **Objective:** To provide training in the elucidation of molecular structures using spectroscopic methods.

10. Details of Course:

S. No.	Contents	Contact Hours
1.	**Electronic Spectroscopy**: Absorption, electronic transitions in inorganic and organic molecules, charge transfer transitions in organic and inorganic molecules, LMCT and MLCT, d-d transitions, Woodward-Fieser rules for alkenes, Woodward rules for enones and arenes, reflectance spectroscopic techniques.	6
2.	**Emission Spectroscopy**: Fluorescence, delayed fluorescence (TADF & TFDF), fluorescence quantum yield, lifetime, Stokes shift, solvent effects, types of quenching with kinetics, energy transfer mechanisms, electron transfer mechanisms, inter-system crossing, phosphorescence, aggregation-induced emission, photochromism, photo catalysis, photodynamic therapy, light-emitting cells.	10
3.	**IR and Raman Spectroscopy**: Active modes of vibrations, survey of functional groups in organic and inorganic compounds, effect of isotopic substitution, conjugation and symmetry; ATR and DRIFTS techniques; Raman	8
4.	**Nuclear Magnetic Resonance Spectroscopy**: Features of ^{1}H NMR spectrum, chemical shifts, spin-spin couplings, coupling constants, dependence of J on dihedral angle, analysis of first order spectra and complex multiplets, chemical and magnetic equivalence and second order effects, OH/NH and dynamic processes, off-resonance decoupling, ^{13}C and other heteronuclei NMR spectra, NOE effects, chemical shift reagents, correlation spectroscopy, NMR of paramagnetic compounds, solid state NMR, simulation of NMR.	12
5.	**Electron Spin Resonance Spectroscopy**: Line shapes, isotropic and anisotropic interactions, theory of g-factors & hyperfine interactions, features of EPR spectra of metal complexes, structural information from EPR spectra of complexes, simulation of EPR.	6
	Total	42

11. Suggested Books:

S. No.	Name of Authors/ Books/ Publishers	Year of Publication /Reprint
1.	Pavia, D. L., Lampman, G.M., Kriz, G. S., "Introduction to Spectroscopy", 5th Ed., Cengage Learning India Private Limited, New Delhi.	**2015**
2.	Kemp, W., "Organic spectroscopy", 3rd Ed, Macmillan, New York.	**2011**
3.	Crews, P., Rodríguez, J., Jaspars, M., "Organic structure analysis", 2nd Ed, Oxford University Press, Oxford.	**2010**
4.	Williams D. H., Flemming, I., "Spectroscopic methods in organic chemistry" , 6th Ed, Mc Graw Hill.	**2011**
5.	Silverstein, R. M., Webster, F. X., Kiemle, D. J., Bryce, D. L., Spectrometric identification of organic compounds", 8th Ed, Wiley.	**2014**
6.	Weil, J. A., Bolton, J. R., "Electron paramagnetic resonance: Elementary theory and practical applications", 2nd Ed, John Wiley & Sons Inc.	**2007**