

## CA S 414: INORGANIC SPECTROSCOPY AND OPTICAL METHODS

### Course Outcomes

- Students will learn the basic principles and applications of ESR and Mossbauer spectroscopy.
- Students can be familiarizing with NQR and Photoelectron spectroscopy.
- Students will gain knowledge on Atomic Absorption Spectrometry, Emission Spectroscopy, Molecular Luminescence Spectroscopy and Light-Scattering methods for detection of metals, particles and particle size.
- Overall students can solve the problems related to above mentioned analytical techniques.

### UNIT-I

[12 Hours]

**Electron Spin Resonance (ESR) Spectroscopy:** Basic principles, selection rules, intensity, width, position of spectral line, multiplet structure of ESR spectra, hyperfine interaction, spin-orbit coupling, Zero Field splitting and Kramer's degeneracy, rules for interpreting spectra, factors affecting the magnitude of values. Instrumentation; Applications to the study simple inorganic and organic free radicals and to inorganic complexes, biological studies and rate of electron exchange reactions.

**Mössbauer Spectroscopy:** The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, Application to the study of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  compounds,  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$  compounds (nature of M-L bond, coordination number and structure), structure determination of  $\text{Fe}_3(\text{CO})_{12}$ , Prussian blue, oxyhemerythrin, hexacyanoferrates, nitroprusside, tin halides. Detection of oxidation states and inequivalent Mössbauer atoms.

### UNIT-II

[12 Hours]

**Nuclear Quadrupole Resonance (NQR) Spectroscopy:** Basic concepts-Nuclear electric quadrupole moment, electric field gradient, energy levels and NQR frequencies, effect of magnetic field on spectra; Factors affecting the resonance signal-Line shape, position of resonance signal; Relationship between electric field gradient and molecular structure. Interpretation of NQR data, structural information of  $\text{PCl}_5$ ,  $\text{TeCl}_4$ ,  $\text{Na}^+ \text{GaCl}_4^-$ ,  $\text{BrCN}$ ,  $\text{HIO}_3$  and Hexahalometallates.

**Photoelectron Spectroscopy:** Basic principles, photoionization process, ionization energies, Koopman's theorem, Electron spectroscopy for chemical analysis (ESCA)-Photoelectron spectra of simple molecules- $\text{N}_2$ ,  $\text{O}_2$  and  $\text{F}_2$ ; Photoelectron spectra for the isoelectronic sequence-Ne, HF,  $\text{H}_2\text{O}$ ,  $\text{NH}_3$  and  $\text{CH}_4$ ; chemical information from ESCA.

**X-ray photoelectron and Auger electron spectroscopy:** Principles and applications. Auger transitions, measurement techniques. Applications.

**Flame Photometry:** Flame emission spectroscopy (FES) and atomic absorption spectroscopy (AAS)-Introduction, principle, flames and flame spectra, variation of emission intensity with the flame, flame temperature, chemical reactions in flame, metallic spectra in flame, flame background. Total consumption and premix burners, role of temperature on absorption, emission and fluorescence. Effect of organic solvents. Comparative study of the basic components and difference in the instrumental design for atomic absorption and flame photometry. Precision and accuracy of AAS and FES. Relationship between AAS and FES, advantages over FES, devices used for the formation of an atomic vapour, applications, determination of sodium in different samples by flame photometry. Plasma emission spectroscopy-Principle, Inductively coupled plasma emission (ICP). ICP torch, instrumentation and applications.

### References

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3. Analytical Chemistry, 6<sup>th</sup> edn., G. D. Christian, Wiley-India (2015).
4. Analytical Chemistry, 4<sup>th</sup> edn., G. D. Christian, John Wiley & Sons (1986).
5. Instrumental methods of analysis, 7<sup>th</sup> edn., H. H. Willard, L. L. Merritt and J. J. Dean, Wadsworth (2012).
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7. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Ranklin and S. Cradock, Blackwell Scientific (1991).
8. Spectroscopy in Inorganic Chemistry: Vol I & II, C. N. R. Rao and J. R. Ferraro, Academic Press (1970).
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14. Instrumental methods of Chemical Analysis, 5<sup>th</sup> edn., Gurdeep R. Chatwal, Himalaya Publishing House (2015).
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