Government PG College, Ambala Cantt

Course File (Session 2023-24)

Name of Professor: Dr. Harneet Kaur

Class: BSc-II/4th Semester/ SECTION: NM

Subject code and Name: PH-602, Paper – XII, Atomic and Molecular Spectroscopy

SYLLABUS

Maximum Marks: 40 **Internal: 10**

Time: 3 hours

Note: The syllabus is divided into 4 units. 9 questions will be set. Question no 1 will be compulsory, it contains 6 parts (form all the four units) and answer should be brief but not in yes / no. Four more questions are to be attempted, selecting one question from each unit. Questions 2-9 may contain two or more parts. All questions carry equal marks. 20% numerical problems are to be set. Use of scientific (non-programmable) calculator is allowed

Syllabus

Unit – I: Historical background of atomic spectroscopy

Introduction of early observations, emission and absorption spectra, atomic spectra, wave number, spectrum of Hydrogen atom in Balmer series, Bohr atomic model(Bohr's postulates) , spectra of Hydrogen atom , explanation of spectral series in Hydrogen atom, un-quantized states and continuous spectra, spectral series in absorption spectra, effect of nuclear motion on line spectra (correction of finite nuclear mass), variation in Rydberg constant due to finite mass, short comings of Bohr's theory, Wilson sommerfeld quantization rule, de-Broglie interpretation of Bohr quantization law, Bohr's corresponding principle, Sommerfeld's extension of Bohr's model, Sommerfeld relativistic correction, Short comings of Bohr-Sommerfeld theory, Vector atom model; space quantization, electron spin, coupling of orbital and spin angular momentum, spectroscopic terms and their notation, quantum numbers associated with vector atom model, transition probability and selection rules.

Unit –II: Vector Atom Model (single valance electron)

Orbital magnetic dipole moment (Bohr megnaton), behavior of magnetic dipole in external magnetic filed; Larmors' precession and theorem. Penetrating and Non-penetrating orbits, Penetrating orbits on the classical model; Quantum defect, spin orbit interaction energy of the single valance electron, spin orbit interaction for penetrating and non-penetrating orbits. quantum mechanical relativity correction, Hydrogen fine spectra, Main features of Alkali Spectra and their theoretical interpretation, term series and limits, Rydeburg-Ritze combination principle, Absorption spectra of Alkali atoms. observed doublet fine structure in the spectra of alkali metals and its Interpretation, Intensity rules for doublets, comparison of Alkali spectra and Hydrogen spectrum .

UNIT-III: Vector Atom model (two valance electrons)

Essential features of spectra of Alkaline-earth elements, Vector model for two valance electron atom: application of spectra. Coupling Schemes;LS or Russell – Saunders Coupling Scheme and JJ coupling scheme, Interaction energy in L-S coupling (sp, pd configuration), Lande interval rule, Pauli principal and periodic classification of the elements. Interaction energy in JJ Coupling (sp, pd configuration), equivalent and non-equivalent electrons, Two valance electron system-spectral terms of non-equivalent and equivalent electrons, comparison of spectral terms in L-S And J-J coupling. Hyperfine structure of spectral lines and its origin; isotope effect, nuclear spin.

Unit –IV: Atom in External Field

Zeeman Effect (normal and Anomalous),Experimental set-up for studying Zeeman effect, Explanation of normal Zeeman effect(classical and quantum mechanical), Explanation of anomalous Zeeman effect(Lande g-factor), Zeeman pattern of D1 and D2 lines of Naatom, Paschen-Back effect of a single valence electron system. Weak field Stark effect of Hydrogen atom.

Molecular Physics General Considerations, Electronic States of Diatomic Molecules, Rotational Spectra (Far IR and Microwave Region), Vibrational Spectra (IR Region), Rotator Model of Diatomic Molecule, Raman Effect, Electronic Spectra.

References

1 Beiser A, Concept of Modern Physics (1987), Mc Graw Hill Co Ltd, New Delhi

2 Rajab J B, Atomic Physics (2007), S Chand & Co, New Delhi

3 Fewkes J H and Yarwood J Atomic Physics Vol II (1991) Oxford University Press

4 Bransden B H and Joachain C J, Physics of Atoms and Molecules 2nd Ed (2009),

Pearson Education, New Delhi.

5 Banwell, Molecular Spectroscopy

6 Ghoshal S N, Atomic and Nuclear Physics Vol I (1996) S Chand & Co, New Delhi

7 Gopalkrishnan K, Atomic and Nuclear Physics (1982), Mc Millan India New Delhi

8 Raj Kumar, Atomic and Moleculer Spectra:Laser , Kedarnath Ram nathpub.

9 S.L.Gupta, V.Kumar,R.C.Sharma, Elements of Spectroscopy,Pragati Prakashan

COURSE OBJECTIVES

The course objectives outlined are as follows:

- **Historical Background and Fundamental Principles:** Understand the historical development of atomic spectroscopy, from early observations to Bohr's atomic model. Gain insights into the concepts of atomic spectra, wave numbers, and the behavior of hydrogen atoms.
- **Quantum Mechanical Models**: Comprehend the Bohr atomic model, Sommerfeld's extension, and the Vector Atom Model. Learn about electron spin, space quantization, and spectroscopic terms associated with quantum mechanics.
- **Analysis of Single Valence Electron Systems:** Explore the Vector Atom Model for single valence electron systems, including orbital magnetic dipole moments, spin-orbit interactions, and fine structure in alkali spectra. Understand the theoretical interpretation of alkali spectra and absorption phenomena.
- **Analysis of Two Valence Electron Systems:** Study the Vector Atom Model for two valence electron systems, coupling schemes (LS and JJ coupling), and spectral terms associated with equivalent and non-equivalent electrons. Explore hyperfine structure and its origin, including the isotope effect and nuclear spin.
- **Atom in External Fields:** Investigate the Zeeman effect (normal and anomalous), Paschen-Back effect, and Stark effect. Understand the experimental setups for studying these effects and their implications for atomic behavior in external fields.
- **Introduction to Molecular Physics**: Gain an overview of molecular physics, including electronic states of diatomic molecules, rotational and vibrational spectra, the rotator model, Raman effect, and electronic spectra. Understand the general considerations and experimental techniques in molecular physics.

By the end of the course, students will have acquired a comprehensive understanding of the principles and applications of atomic and molecular spectroscopy, enabling them to analyze and interpret complex spectra, understand atomic behavior in external fields, and apply spectroscopic techniques to various scientific and technological fields.

COURSE OUTCOMES:

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

- Acquire knowledge about the historical background and developments of atomic spectroscopy through the study of spectral series in Hydrogen atom.
- Effect of nuclear motion on line spectra (correction of finite nuclear mass), short comings of Bohr's theory
- Wilson sommerfeld quantization rule, Sommerfeld's extension of Bohr's model, Sommerfeld relativistic correction, Short comings of Bohr-Sommerfeld theory
- Vector atom model.
- Understand and explain the vector atom model, various coupling schemes and atomic spectra of one and two electron atoms.
- Explain the influence on the spectra of atoms in the presence of external applied electric and magnetic field i.e. Zeeman effect, Paschen-Back effect, Stark effect.
- Have basic idea about the rotational, vibrational and rotational-vibrational spectra of diatomic molecules and basic idea of Raman Effect

Lesson Plan

Week No.	Scheduled Dates	Topics to be covered
1.	8th Jan 2024-13th Jan2024	**Unit-I: Historical background of atomic spectroscopy**Introduction of early observations, emission and absorption spectra, atomic spectra, wave number, spectrum of Hydrogen atom in Balmer series, Bohr atomic model(Bohr's postulates).
2.	15th Jan 2024-20th Jan2024	Spectra of Hydrogen atom , explanation of spectral series in Hydrogen atom, un-quantized states and continuous spectra spectral series in absorption spectra, effect of nuclear motion on line spectra, variation in Rydberg constant due to finite mass, short comings of Bohr's theory
3.	22th Jan 2024-27th Jan2024	Wilson sommerfeld quantization rule, de-Broglie interpretation of Bohr quantization law, Bohr's corresponding principle, Sommerfeld's extension of Bohr's model, Sommerfeld relativistic correction, Short comings of Bohr-Sommerfeld theory.
4.	29th Jan 2024-3rd Feb2024	Space quantization, electron spin, coupling of orbital and spin angular momentum, spectroscopic terms and their notation, quantum numbers associated with vector atom model, transition probability and selection rules. **Class Test, Revision and doubts of unit-1**
5.	5th Feb 2024- 10th Feb 2024	**Unit –II: Vector Atom Model (single valance electron)**Orbital magnetic dipole moment (Bohr megnaton), behaviour of magnetic dipole in external magnetic field; Larmors' precession and theorem
6.	12th Feb 2024- 17th Feb 2024	Penetrating and Non-penetrating orbits, Penetrating orbits on the classical model. Quantum defect, spin orbit interaction energy of the single valance electron, spin orbit interaction for penetrating and non-penetrating orbits.
7.	19th Feb 2024- 24th Feb 2024	quantum mechanical relativity correction, Hydrogen fine spectra, Main features of Alkali Spectra and their theoretical interpretation, term series and limits, Rydeburg-Ritze combination principle, Absorption spectra of Alkali atoms.
8.	26th Feb 2024- 2nd March 2024	observed doublet fine structure in the spectra of alkali metals and its interpretation, Intensity rules for doublets, comparison of Alkali spectra and Hydrogen spectrum.

		Class test, Revision and doubts of unit-2
9.	4th March 2024-9th March 2024	**UNIT-III: Vector Atom model (two valance electrons)** Essential features of spectra of Alkaline-earth elements, Vector model for two valance electron atom: application of spectra, LS and JJ Coupling Scheme
10.	11th March 2024-16th March 2024	Interaction energy in L-S coupling (sp, pd configuration), Lande interval rule, Pauli principal and periodic classification of the elements, Interaction energy in JJ Coupling (sp, pd configuration
11.	18th March 2024-22nd March 2024	Equivalent and non-equivalent electrons and their spectral terms, Comparison of spectral terms in L-S And J-J coupling. Hyperfine structure of spectral lines and its origin; isotope effect, nuclear spin. **Revision and doubts of unit-3**
	23rd March 2024 to 31st March 2024	Holi Break
12.	1st April 2024 to 6th April 2024	**Unit –IV: Atom in External Field** Zeeman Effect (normal and Anomalous), Experimental set-up for studying Zeeman effect, Explanation of normal Zeeman effect(classical and quantum mechanical)
13.	8th April 2024 to 13th April 2024	Explanation of anomalous Zeeman effect (Lande g-factor), Zeeman pattern of D1 and D2 lines of Na atom, Paschen-Back effect of a single valence electron system. Weak field Stark effect of Hydrogen atom
14.	15th April 2024 to 20th April 2024	General considerations of molecular spectra, Electronic States of Diatomic Molecules, Rotational Spectra (Far IR and Microwave Region), Vibrational Spectra (IR Region)
15.	22th April 2024 to 27th April 2024	Rotator Model of Diatomic Molecule, Raman Effect, Electronic Spectra, **Revision and doubts of unit-4**
16.	29th April 2024 to 30th May 2024	Revision : Doubts and Discussion, Previous years question papers