Lahore University of Management Sciences

CHEM 221/PHY335 – Molecular Symmetry I

Fall 2023

Instructor	Ghayoor Abbas
Room No.	9-415A
Office Hours	TBD
Email	ghayoor.abbas@lums.edu.pk
Telephone	3560-8281
Secretary/TA	TBD
TA Office Hours	TBD
Course URL (if any)	

Course Basics				
Credit Hours	3			
Lecture(s)	Nbr of Lec(s) Per Week	2	Duration	1 hr & 15 minutes
Recitation/Lab (per week)	Nbr of Lec(s) Per Week	NA	Duration	NA
Tutorial (per week)	Nbr of Lec(s) Per Week	NA	Duration	NA

Course Distribution	
Core	Chemistry Core
Elective	NA
Open for Student Category	SBASSE
Close for Student Category	NA

COURSE DESCRIPTION

This course covers fundamentals of inorganic chemistry including shapes of orbitals, electronic configurations, orbital energies, periodic trends, chemical bonding etc. Students will be introduced with the basics of main group chemistry and coordination chemistry. The second part of this course will provide a systematic presentation of the chemical applications of group theory with emphasis on the formal development of the subject and its applications to the physical methods of inorganic chemical compounds. Course will conclude on Solid state chemistry, and if possible acid base chemistry.

COURSE PREREQUISITE(S)

- CHEM 101 or Consent of instructor

COURSE OBJECTIVES

- To study orbital shapes, electronic configurations.
- To correlate orbital energies with periodicity (Ionization energy, electron affinity etc.).
- To discuss chemistry of main group elements.
- To introduce various geometries of transition metal complexes and possible isomerism
- To identify various symmetry elements (axis, plane, rotation-reflection, inversion) present in a given molecule or structure.
- Assignment of (correct) point groups to a given molecule or shape.
- Form a non-degenerate representation to describe the effect of symmetry operations.
- Reduce the non-degenerate representation to its component irreducible representations.
- Apply the principles of symmetry & group theory to solve simple problems in chemical bonding, molecular vibrations, and electronic spectra of transition metal complexes.

	Basic concepts of coordination chemistry, acid-base chemistry, and solid state chemistry.

Learning Outcomes	
	After completing this course successfully, the student is expected to: • Determine the shapes of molecules using VSEPR or VBT. • Predict the geometry and isomers of a given metal complex • Recognize various symmetry elements (axis, plane, rotation-reflection, inversion) present in a given molecule or structure. • Based on the symmetry elements present, state the point group to which a given molecule belongs. • Form a non-degenerate representation to describe the effect of symmetry operations. • Reduce the non-degenerate representation to its component irreducible representations. • Set-up a matrix to perform a given transformation. • Find the character of a matrix representing a symmetry operation, using any given basis. Applications to chemical bonding and spectroscopy: ▪ Finding sets of hybrid orbitals with given directional properties ▪ Determining the orbitals suitable for pi-bonding ▪ Finding the symmetries of LCAO molecular orbitals ▪ Constructing simple molecular orbital correlation diagrams ▪ Finding the number of IR or Raman active vibrations ▪ Determining splitting of orbitals in a given environment ▪ Electronic spectra of transition metal complexes. • Differentiate between hard and soft acids and bases • Understand crystal systems, calculate number of atoms per unit cell

Grading Breakup and Policy
Assignment(s): 0%; 4-5 Assignments will be given. Home Work: Quiz(s): 20% 5-7 quizzes will be given. All quizzes given will count towards this instrument of the grade. Class Participation: 0% All students are strongly encouraged to actively participate in class discussions. Attendance: Students are required to attend and actively participate in all the classes. Less than 90% attendance will result in F grade. Midterm Examination: 40% Project: 0% Final Examination: 40% I can change the grading breakup up to ±5%.

Examination Detail	
Midterm Exam	Yes/No: Yes Combine Separate: NA Duration: 3 hr Preferred Date: TBD Exam Specifications: Closed Books, Closed Notes, Calculators allowed
Final Exam	Yes/No: Yes Combine Separate: NA Duration: 3 hr Exam Specifications: Closed Books, Closed Notes, Calculators allowed

Lahore University of Management Sciences

COURSE OVERVIEW			
Week/ Lecture/ Module	Topics	Recommended Readings	Objectives/ Application
1-2	Introduction to Inorganic Chemistry, shapes of orbitals, electronic configurations and the periodic table, orbital energies and the effective nuclear charges, ionization energy, electron affinity, Trends in Oxidation states.	Chapter 8 Keeler & Wothers Chapter 1 Catherine E. Housecroft Chapter 3 Miessler & Tarr	To learn electronic configuration and periodic trends.
2-3	Bonding in the elements, non-metals, metallic structures, transition from metals to non-metals. Bonding between the elements, Effect of orbital size and energy mismatch, classification of compounds as ionic or covalent, Structural trends across the periodic table, radius ratio rules, compounds with lower coordination numbers.	Chapter 9 Keeler & Wothers	
4-5	Main-group chemistry, Overview, key concepts in main group chemistry, hydrolysis of chlorides, oxides, brief survey of chemistry of each group	Chapter 16 Keeler & Wothers Chapter 10-18 Catherine E. Housecroft Chapter 8 Miessler & Tarr	To compare the chemical and physical properties of the second period main-group elements with the properties of the heavier elements in the same groups.
6-7	Transition metals, orbital energies and oxidation states, complexes, Structure & Geometry of Transition Metal Complexes, isomerism, bonding, high-spin and low-spin octahedral complexes, magnetic and spectroscopic properties, consequences of splitting of d orbitals, tetrahedral and square-planar complexes, aqueous chemistry and oxo-anions	Chapter 17 Keeler & Wothers	
8	Symmetry elements and operations	Chapter 3 Keeler & Wothers Program 1: Alan Vincent	To Identify symmetry elements and operations present in a given molecule. To assign point groups.
9	Point groups	Program 2: Alan Vincent	To assign point groups.
10	Non-degenerate Representations, Matrices, Degenerate Representations	Program 3: Alan Vincent Program 4: Alan Vincent Program 6: Alan Vincent	Form non-degenerate representations to describe the effect of symmetry operations, Reduction of reducible representations Set up matrix to perform a given transformation Degenerate Representations
11-12	Applications of Symmetry VBT & MOT	Chapter 5 Keeler & Wothers Program 6 & 7: Alan Vincent	Applications of Symmetry and group theory in chemistry

13-14	Acid Base and Solid state Chemistry	Chapter 6 Keeler & Wothers Chapter 6 Catherine E. Housecroft Chapter 7 Miessler & Tarr	Crystals systems, Unit Cell, # of particles per unit cell

Textbook(s)/Supplementary Readings

Text Books

- Chemical Structure and Reactivity an Integrated Approach by James Keeler & Peter Wothers, 2nd Edition, 2014, Oxford.
- Molecular Symmetry & Group Theory by Alan Vincent, 2nd Edition, 2001, John Wiley and Sons.
- Inorganic Chemistry by Mark Weller, Jonathan Rourke, Tina Overton, & Fraser Armstrong, 7th Edition, 2018, Oxford
- Inorganic Chemistry by Catherine E. Housecroft & Alan G. Sharpe, 5th Edition, 2018, Pearson.

Supplementary Readings

- Inorganic Chemistry by Gary L. Miessler & Donald A. Tarr, 5th Edition, 2014, Pearson.
- Molecular Symmetry & Group Theory, by Robert L Carter, 2004, John Wiley and Sons.
- Chemical Applications of Group Theory, F. Albert Cotton, 3rd Edition, 1999, John Wiley and Sons.

Additional Notes

Molecular Models: Molecular models will be of great help for concepts related to symmetry. Students are strongly encouraged to use molecular models to understand various symmetry elements and operations.

Web Resources: Several web resources available, the following are representative.

http://symmetry.otterbein.edu/

http://web.mit.edu/5.03/www/

http://ocw.mit.edu/courses/chemistry/5-04-principles-of-inorganic-chemistry-ii-fall-2008/index.htm

http://csi.chemie.tu-darmstadt.de/ak/immel/script/redirect.cgi?filename=http://csi.chemie.tu-darmstadt.de/ak/immel/tutorials/symmetry/index.html

http://www.staff.ncl.ac.uk/j.p.goss/symmetry/index.html