

Course Outline

Chemistry 9571, Winter 2026

1. Course Information

Course number: **9571**

Course Title: ***Vibrational Spectroscopy of Solid-state Materials***

Lectures / seminars:

Day/s: TBA

Time/s: TBA

Mode of instruction: In person

2. Enrollment Restrictions

No limit

3. Instructor Information

Instructor:

Name: Yining Huang

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4. Course Description and Graduate Course Level Learning Outcomes/Objectives

Course Description

Infrared (IR) and Raman spectroscopy are complementary techniques widely used for the structural characterization of materials. While the theoretical relationship between molecular geometry, symmetry, and the number of IR and Raman active modes is well established, this connection is often not clear to many researchers and students in practical spectral interpretation, particularly for solids, where spectra differ significantly from those of molecules in the gas or liquid phases.

This course introduces a systematic approach to understanding vibrational spectra of solid-state materials. It begins with a brief review of molecular vibrations and point group theory for free molecules, followed by an introduction to solid-state effects. Topics include site symmetry, intermolecular interactions, and correlation field (factor group) analysis to explain changes in the number, activity, and splitting of vibrational modes in crystalline solids.

Learning Outcomes

By the end of this course, students will be able to:

1. Apply group theory to determine vibrational modes and IR/Raman activity of free molecules using point group analysis.
2. Relate molecular geometry and symmetry to vibrational spectra.
3. Interpret IR and Raman spectra of crystalline solids, accounting for solid-state effects such as intermolecular interactions and symmetry reduction.
4. Use site symmetry and factor group analysis to predict the number, activity, and splitting of vibrational modes in molecular crystals.
5. Distinguish molecular and lattice vibrations and assess their contributions to solid-state spectra.
6. Critically analyze experimental spectra and connect spectral features to crystal structure.

5. Topics:

1. Molecular symmetry
 - a. Symmetry elements and operations
 - b. Point groups
2. Vibrational spectroscopy
 - a. Infrared adsorption and Raman scattering
 - b. Character tables
 - c. The number and activity of vibrations for an isolated molecules (in gas phase and solution)
3. Vibrational spectra of solids
 - a. Crystal symmetry
 - b. Solid-state effects
 - c. Selection rules for vibrational spectra of solids (factor group analysis)
 - d. External modes
 - e. Applications and special cases

6. Course Materials

There is no required textbook. Lecture notes will be provided.

7. Methods of Evaluation

Assignments 60%

Exam (open book) 40%

Note: The use of artificial intelligence (AI) tools is **not** permitted in assessments or the final examination.

8. Statement on Academic Offences

Scholastic offences are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following website:

https://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_offences.pdf

9. Health/Wellness Services

Students who are in emotional/mental distress should refer to Mental Health Support at <https://www.uwo.ca/health/psych/index.html> for a complete list of options about how to obtain help.

10. Accessible Education (AE)

Western is committed to achieving barrier-free accessibility for all its members, including graduate students. As part of this commitment, Western provides a variety of services devoted to promoting, advocating, and accommodating persons with disabilities in their respective graduate program.

Graduate students with disabilities (for example, chronic illnesses, mental health conditions, mobility impairments) are strongly encouraged to register with Accessible Education (AE), a confidential service designed to support graduate and undergraduate students through their academic program. With the appropriate documentation, the student will work with both AE and their graduate programs (normally their Graduate Chair and/or Course instructor) to ensure that appropriate academic accommodations to program requirements are arranged. These accommodations may include individual counselling, alternative formatted literature, accessible campus transportation, learning strategy instruction, writing exams and assistive technology instruction.

11. Statement on Gender-Based and Sexual Violence

Western is committed to reducing incidents of gender-based and sexual violence (GBSV) and providing compassionate support to anyone who is going through or has gone through these traumatic events. If you are experiencing or have experienced GBSV (either recently or in the past), you will find information about support services for survivors, including emergency contacts at the following website: https://www.uwo.ca/health/student_support/survivor_support/get-help.html

To connect with a case manager or set up an appointment, please contact support@uwo.ca.

12. Statement on the Use of Generative Artificial Intelligence (AI)

Unless otherwise stated, the use of generative AI tools (e.g., ChatGPT, Microsoft Copilot, Google Gemini, or similar platforms) is not permitted in the completion of assignments, and final examinations.