

University of Western Ontario  
Chemistry 9754R, Fall 2024 (Oct 24 – Dec 5)  
**Powder Diffraction**

**Instructor:**

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**Description:**

The course addresses structural characterization and quantitative analysis for solid crystalline materials by X-ray powder diffraction techniques. Topics include pattern processing and indexing, data mining, structural visualization, introduction to Rietveld refinement - theory and use of computer software for structural refinement on powder patterns.

**Topics:**

<b>Week</b>	<b>Topic</b>
1	Solid material classifications. Available structural characterization probes. Review of basics of space group and crystallography: definitions, symmetry elements, screw axis, glide plane, 230 space groups, matrix representations, Bravais lattices, reciprocal lattices, 32 crystallography point groups, equivalent sites, international tables for crystallography.
2	Introduction of powder x-ray diffraction. Diffraction theories. Single crystal vs. powder diffraction. Energy dispersive vs. angle dispersive. Instrumentation, pattern acquisition and processing.
3	Pattern indexing. Reflections, d-spacings and Miller indices. General techniques, indexing algorithms, data mining, use of software.
4	Introduction to Rietveld refinement. History and achievements. Principles, algorithms, parameters, quantitative analysis. Limitations.
5	Introduction to Rietveld refinement software: GSAS. Primer for EXPGUI and GSAS. File preparations and extraction of structure. Refinement parameters. Crystal structure visualization.
6	Hands on practice on refinement of powder patterns. Refinement of lanthanum hexaboride powder pattern. Multiple phases and quantitative

**Resources:**

- 1) Course website: <http://owl.uwo.ca/> (requires login with UWO email account).
- 2) Textbook: None. Some recommended reference books will be available from library or online.
- 3) Lecture notes and handouts will be provided via Owl.
- 4) Laptop PC with Windows OS is recommended.

**Lectures / seminars:**

Day/s:           Thursdays

Time/s:          2:30 – 4:30 PM

Mode of instruction: In person

**Evaluation**

Problem sets (3 assignments)   60%

Comprehensive project

## **Health and Wellness**

As part of a successful graduate student experience at Western, we encourage students to make their health and wellness a priority. Western provides several on campus health-related services to help you achieve optimum health and engage in healthy living while pursuing your graduate degree. For example, to support physical activity, all students, as part of their registration, receive membership in Western's Campus Recreation Centre.

Numerous cultural events are offered throughout the year. For example, please check out the Faculty of Music web page <http://www.music.uwo.ca/>, and our own McIntosh Gallery <http://www.mcintoshgallery.ca/>. Information regarding health- and wellness-related services available to students may be found at <http://www.health.uwo.ca/>. Students seeking help regarding mental health concerns are advised to speak to someone they feel comfortable confiding in, such as their faculty supervisor, their program director (graduate chair), or other relevant administrators in their unit. Campus mental health resources may be found at [http://www.health.uwo.ca/mental\\_health/resources.html](http://www.health.uwo.ca/mental_health/resources.html).

## **Use of Generative Artificial Intelligence (AI)**

The use of generative artificial intelligence (AI) tools/software/apps is acceptable, and permitted in the course as long as such use is appropriately disclosed with sufficient details provided.