X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
Two individual assignments *include independent data collection for at least two different crystalline materials. This will be done outside of scheduled class times. Students are required to arrange for use of instruments not later than halfway through the semester, after the student has passed the Online X-ray Safety Training and Quiz for Analytical X-ray Equipment. The origin of the material can be with the student, or a sample can be provided. Where possible, the materials (molecular organic and metal organic compounds, metallic or ceramic solid state materials) will be matched to the research background of the student. Ideally, the material's structure should be unknown and not yet reported. The assignment will involve crystal selection, data collection and processing, structure solution, refinement and validation. The final report should consist of the cif and res file. The exact grade fraction of each assignment will depend on the number and complexity of the individual assignments given out.*

Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
Take home assignment 12, Individual Lab Assignment 2	*200*
Total (40% of total grade)	*1265*

Midterm. 20%
*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

Lab-Practical: 20%
*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

Final. 20%
*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
The ultimate goal of this class is for students to be able to independently use the learned material for analysis of their own samples relating to their research. This part, while necessarily less reflected in the overall grade, relies heavily on engaged participation in the lab section of the class.

Policies

General Course Policies

(1) Students are welcome to ask questions outside of class and lecture times, either in person or via e-mail. Phone or text inquiries are likely to be missed or ignored.
(2) Students are encouraged to hand in assignments two or three days early for a first evaluation and suggestions/pointers for improvements. Assignments handed in on the due day will be graded "as received".
(3) Class starts on time. If you are late or have to leave early do so quietly without interrupting others.
(4) Absolutely no cell phone use in class at any time; cell phones have to "remain dark and silent" during the entire class period.
(5) Use of computers in class is limited to assigned work related to class; no use of social networks; no use of internet other than required for class.

Grading

A+	97%-100%	4.33/4.00
A	93%-96%	4.00/4.00
A-	90%-92%	3.67/4.00
B+	87%-89%	3.33/4.00
B	83%-86%	3.00/4.00
B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

Academic Dishonesty

Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Part 5, Section III-B-2-a, Student Regulations] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15, 1972]

***Plagiarism**, in the context of this class, includes **use of ANY material without citation of the original source**. Exceptions are solely material from the assigned text books, and material handed out in class. Sources that should be cited are, but are not limited to, peer reviewed publications, books, non-peer reviewed publications, online*

sources, technical and procedural manuals, and personal communications from others. Use of incorrect material, even if publicly accessible, does not qualify as waiver for wrongly answered questions (exception: peer reviewed indexed publications).

Please also refer to Purdue's student guide for academic integrity:
https://www.purdue.edu/odos/academic-integrity/

Use of Copyrighted Materials
Students are expected, within the context of the Regulations Governing Student Conduct and other applicable University policies, to act responsibly and ethically by applying the appropriate exception under the Copyright Act to the use of copyrighted works in their activities and studies. The University does not assume legal responsibility for violations of copyright law by students who are not employees of the University.

A Copyrightable Work created by any person subject to this policy primarily to express and preserve scholarship as evidence of academic advancement or academic accomplishment. Such works may include, but are not limited to, scholarly publications, journal articles, research bulletins, monographs, books, plays, poems, musical compositions and other works of artistic imagination, and works of students created in the course of their education, such as exams, projects, theses or dissertations, papers and articles.

Please also refer to the University Regulations on policies:
http://www.purdue.edu/policies/academic-research-affairs/ia3.html

Attendance
Students are expected to be present for every meeting of the class. Regular attendance is essential for successfully completing this course. However, no attendance will be taken and excuses will only be required for the dates of mid-term, lab practical and final. Students are required to independently make up missed course sections, and to inquire about assignments if they miss a lecture or lab. When conflicts or absences can be anticipated for the dates of mid-term, lab practical and final, such as for University sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible so that possibly a different date can be scheduled for the test. For unanticipated or emergency absences when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, or by contacting the main chemistry office. When the student is unable to make direct contact with the instructor and is unable to leave word with the department because of circumstances beyond the student's control, and in cases of bereavement, the student or the student's representative should contact the Office of the Dean of Students.

The link to the Purdue's complete policy and implications can be found at:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Missed or Late Work
Homework assignments handed in late will not be accepted (exception: unanticipated or emergency absences, see "Attendance", above). An assignment handed in after the due day 5 pm will incur a zero-point grade.

If a student misses a take home assignment, mid-term, lab practical or final due to unanticipated or emergency absences (see "Attendance", above) a make-up date can be scheduled at the earliest possible date. Unexcused absences incur a zero-point grade.

Grief Absence Policy for Students
Below is the University's Grief Absence Policy for Students:

Purdue University recognizes that a time of bereavement is very difficult for a student. The University therefore provides the following rights to students facing the loss of a family member through the Grief Absence Policy for Students (GAPS). GAPS Policy: Students will be excused for funeral leave and given the opportunity to earn equivalent credit and to demonstrate evidence of meeting the learning outcomes for missed assignments or assessments in the event of the death of a member of the student's family.

See the University's website for additional information:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Violent Behavior Policy
Below is Purdue's policy prohibiting violent behavior:

Purdue University is committed to providing a safe and secure campus environment for members of the university community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent Behavior impedes such goals. Therefore, Violent Behavior is prohibited in or on any University Facility or while participating in any university activity.

See the University's website for additional information:
http://www.purdue.edu/policies/facilities-safety/iva3.html

Mental Health Syllabus Statement

· On the recommendation of the University Senate, CAPS and the Dean the following resources are included in the syllabus.

- **If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack,**

https://purdue.welltrack.com/. Sign in and find information and tools at your fingertips, available to you at any time.

- **If you need support and information about options and resources**, please see the Office of the Dean of Students, http://www.purdue.edu/odos, for drop-in hours (M-F, 8 am- 5 pm).
- **If you're struggling and need mental health services**: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and http://www.purdue.edu/caps/ during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

Emergencies

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

See the University's website for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

Students with Disabilities

The course requires the use of optical microscopes, technical equipment that requires standing and visual alignment of samples, and use of computers in class and for homework assignments and tests. If you have a condition that makes it impossible or difficult to do any of the assigned work then please see the instructor to discuss possible solutions, workarounds or assistance. Academic accommodation must be arranged for BY THE STUDENT through Purdue's Disability Resource Center. The instructor cannot make academic accommodations without a DRC accommodation letter.

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: ***drc@purdue.edu*** *or by phone: 765-494-1247." http://www.purdue.edu/drc/faculty/syllabus.html*

Assistance with Making Learning Materials Accessible. *Purdue's new Innovative Learning group website includes:*

- *Information on Universal Design for learning*
- *Includes our Create Accessible Documents webpage:*

- *How-to training videos and step-by-step documents for faculty to train themselves in making their own course documents accessible*
- *Self-check checklists for evaluation of their own formatting work*
- *Request in-person training on formatting documents*
- *Direct link to request Document Formatting Assistance. The team has 10 student workers ready to assist, and all work is completed in the order it is received.*

Diversity & Inclusion

Purdue University is committed to maintaining an inclusive community that recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, Purdue University seeks to develop and nurture its diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas and enriches campus life.

Purdue University views, evaluates and treats all persons in any university-related activity or circumstance in which they may be involved solely as individuals on the basis of their own personal abilities, qualifications and other relevant characteristics.

Purdue University does not condone and will not tolerate Discrimination against any individual on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, disability, status as a veteran, marital status, parental status, sexual orientation, gender identity or gender expression. Purdue University promulgates policies and programs to ensure that all persons have equal access to its employment opportunities and educational programs, services and activities. The principal objective of this policy is to provide fair and consistent treatment for all students and employees of the University. Purdue is committed to increasing the recruitment, selection and promotion of faculty and staff at the University who are racial or ethnic minorities, women, persons with disabilities and veterans. The University also is committed to policies and programs that increase the diversity of the student body.

Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
http://www.purdue.edu/studentregulations/equal_opportunity/studentgrievance.html
https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic

excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life.

Purdue University prohibits discrimination against any member of the University community on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, marital status, parental status, sexual orientation, gender identity and expression, disability, or status as a veteran. The University will conduct its programs, services and activities consistent with applicable federal, state and local laws, regulations and orders and in conformance with the procedures and limitations as set forth in Executive Memorandum No. D-1, which provides specific contractual rights and remedies. Any student who believes they have been discriminated against may visit www.purdue.edu/report-hate to submit a complaint to the Office of Institutional Equity. Information may be reported anonymously.

Please refer to Purdue's nondiscrimination statement:
http://www.purdue.edu/purdue/ea_eou_statement.html

Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

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Learning Outcomes

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- *Knowledge of the process of crystal structure analysis.*
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Total (40% of total grade)	*1265*

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B	83%-86%	3.00/4.00
B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

Academic Dishonesty

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Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
Two individual assignments *include independent data collection for at least two different crystalline materials. This will be done outside of scheduled class times. Students are required to arrange for use of instruments not later than halfway through the semester, after the student has passed the Online X-ray Safety Training and Quiz for Analytical X-ray Equipment. The origin of the material can be with the student, or a sample can be provided. Where possible, the materials (molecular organic and metal organic compounds, metallic or ceramic solid state materials) will be matched to the research background of the student. Ideally, the material's structure should be unknown and not yet reported. The assignment will involve crystal selection, data collection and processing, structure solution, refinement and validation. The final report should consist of the cif and res file. The exact grade fraction of each assignment will depend on the number and complexity of the individual assignments given out.*

Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
Take home assignment 12, Individual Lab Assignment 2	*200*
Total (40% of total grade)	*1265*

Midterm. 20%
*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

Lab-Practical: 20%
*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

Final. 20%
*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
The ultimate goal of this class is for students to be able to independently use the learned material for analysis of their own samples relating to their research. This part, while necessarily less reflected in the overall grade, relies heavily on engaged participation in the lab section of the class.

Policies

General Course Policies

(1) Students are welcome to ask questions outside of class and lecture times, either in person or via e-mail. Phone or text inquiries are likely to be missed or ignored.
(2) Students are encouraged to hand in assignments two or three days early for a first evaluation and suggestions/pointers for improvements. Assignments handed in on the due day will be graded "as received".
(3) Class starts on time. If you are late or have to leave early do so quietly without interrupting others.
(4) Absolutely no cell phone use in class at any time; cell phones have to "remain dark and silent" during the entire class period.
(5) Use of computers in class is limited to assigned work related to class; no use of social networks; no use of internet other than required for class.

Grading

A+	97%-100%	4.33/4.00
A	93%-96%	4.00/4.00
A-	90%-92%	3.67/4.00
B+	87%-89%	3.33/4.00
B	83%-86%	3.00/4.00
B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
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Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
Two individual assignments *include independent data collection for at least two different crystalline materials. This will be done outside of scheduled class times. Students are required to arrange for use of instruments not later than halfway through the semester, after the student has passed the Online X-ray Safety Training and Quiz for Analytical X-ray Equipment. The origin of the material can be with the student, or a sample can be provided. Where possible, the materials (molecular organic and metal organic compounds, metallic or ceramic solid state materials) will be matched to the research background of the student. Ideally, the material's structure should be unknown and not yet reported. The assignment will involve crystal selection, data collection and processing, structure solution, refinement and validation. The final report should consist of the cif and res file. The exact grade fraction of each assignment will depend on the number and complexity of the individual assignments given out.*

Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
Take home assignment 12, Individual Lab Assignment 2	*200*
Total (40% of total grade)	*1265*

Midterm. 20%
*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

Lab-Practical: 20%
*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

Final. 20%
*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
The ultimate goal of this class is for students to be able to independently use the learned material for analysis of their own samples relating to their research. This part, while necessarily less reflected in the overall grade, relies heavily on engaged participation in the lab section of the class.

Policies

General Course Policies

(1) Students are welcome to ask questions outside of class and lecture times, either in person or via e-mail. Phone or text inquiries are likely to be missed or ignored.
(2) Students are encouraged to hand in assignments two or three days early for a first evaluation and suggestions/pointers for improvements. Assignments handed in on the due day will be graded "as received".
(3) Class starts on time. If you are late or have to leave early do so quietly without interrupting others.
(4) Absolutely no cell phone use in class at any time; cell phones have to "remain dark and silent" during the entire class period.
(5) Use of computers in class is limited to assigned work related to class; no use of social networks; no use of internet other than required for class.

Grading

A+	97%-100%	4.33/4.00
A	93%-96%	4.00/4.00
A-	90%-92%	3.67/4.00
B+	87%-89%	3.33/4.00
B	83%-86%	3.00/4.00
B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

Academic Dishonesty

Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Part 5, Section III-B-2-a, Student Regulations] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15, 1972]

***Plagiarism**, in the context of this class, includes **use of ANY material without citation of the original source**. Exceptions are solely material from the assigned text books, and material handed out in class. Sources that should be cited are, but are not limited to, peer reviewed publications, books, non-peer reviewed publications, online*

sources, technical and procedural manuals, and personal communications from others. Use of incorrect material, even if publicly accessible, does not qualify as waiver for wrongly answered questions (exception: peer reviewed indexed publications).

Please also refer to Purdue's student guide for academic integrity:
https://www.purdue.edu/odos/academic-integrity/

Use of Copyrighted Materials
Students are expected, within the context of the Regulations Governing Student Conduct and other applicable University policies, to act responsibly and ethically by applying the appropriate exception under the Copyright Act to the use of copyrighted works in their activities and studies. The University does not assume legal responsibility for violations of copyright law by students who are not employees of the University.

A Copyrightable Work created by any person subject to this policy primarily to express and preserve scholarship as evidence of academic advancement or academic accomplishment. Such works may include, but are not limited to, scholarly publications, journal articles, research bulletins, monographs, books, plays, poems, musical compositions and other works of artistic imagination, and works of students created in the course of their education, such as exams, projects, theses or dissertations, papers and articles.

Please also refer to the University Regulations on policies:
http://www.purdue.edu/policies/academic-research-affairs/ia3.html

Attendance
Students are expected to be present for every meeting of the class. Regular attendance is essential for successfully completing this course. However, no attendance will be taken and excuses will only be required for the dates of mid-term, lab practical and final. Students are required to independently make up missed course sections, and to inquire about assignments if they miss a lecture or lab. When conflicts or absences can be anticipated for the dates of mid-term, lab practical and final, such as for University sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible so that possibly a different date can be scheduled for the test. For unanticipated or emergency absences when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, or by contacting the main chemistry office. When the student is unable to make direct contact with the instructor and is unable to leave word with the department because of circumstances beyond the student's control, and in cases of bereavement, the student or the student's representative should contact the Office of the Dean of Students.

The link to the Purdue's complete policy and implications can be found at:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Missed or Late Work
Homework assignments handed in late will not be accepted (exception: unanticipated or emergency absences, see "Attendance", above). An assignment handed in after the due day 5 pm will incur a zero-point grade.

If a student misses a take home assignment, mid-term, lab practical or final due to unanticipated or emergency absences (see "Attendance", above) a make-up date can be scheduled at the earliest possible date. Unexcused absences incur a zero-point grade.

Grief Absence Policy for Students
Below is the University's Grief Absence Policy for Students:

Purdue University recognizes that a time of bereavement is very difficult for a student. The University therefore provides the following rights to students facing the loss of a family member through the Grief Absence Policy for Students (GAPS). GAPS Policy: Students will be excused for funeral leave and given the opportunity to earn equivalent credit and to demonstrate evidence of meeting the learning outcomes for missed assignments or assessments in the event of the death of a member of the student's family.

See the University's website for additional information:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Violent Behavior Policy
Below is Purdue's policy prohibiting violent behavior:

Purdue University is committed to providing a safe and secure campus environment for members of the university community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent Behavior impedes such goals. Therefore, Violent Behavior is prohibited in or on any University Facility or while participating in any university activity.

See the University's website for additional information:
http://www.purdue.edu/policies/facilities-safety/iva3.html

Mental Health Syllabus Statement

· On the recommendation of the University Senate, CAPS and the Dean the following resources are included in the syllabus.

- **If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack,**

https://purdue.welltrack.com/. Sign in and find information and tools at your fingertips, available to you at any time.

- **If you need support and information about options and resources**, please see the Office of the Dean of Students, http://www.purdue.edu/odos, for drop-in hours (M-F, 8 am- 5 pm).
- **If you're struggling and need mental health services**: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and http://www.purdue.edu/caps/ during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

Emergencies

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

See the University's website for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

Students with Disabilities

The course requires the use of optical microscopes, technical equipment that requires standing and visual alignment of samples, and use of computers in class and for homework assignments and tests. If you have a condition that makes it impossible or difficult to do any of the assigned work then please see the instructor to discuss possible solutions, workarounds or assistance. Academic accommodation must be arranged for BY THE STUDENT through Purdue's Disability Resource Center. The instructor cannot make academic accommodations without a DRC accommodation letter.

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: ***drc@purdue.edu*** *or by phone: 765-494-1247." http://www.purdue.edu/drc/faculty/syllabus.html*

Assistance with Making Learning Materials Accessible. *Purdue's new Innovative Learning group website includes:*

- *Information on Universal Design for learning*
- *Includes our Create Accessible Documents webpage:*

- *How-to training videos and step-by-step documents for faculty to train themselves in making their own course documents accessible*
- *Self-check checklists for evaluation of their own formatting work*
- *Request in-person training on formatting documents*
- *Direct link to request Document Formatting Assistance. The team has 10 student workers ready to assist, and all work is completed in the order it is received.*

Diversity & Inclusion

Purdue University is committed to maintaining an inclusive community that recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, Purdue University seeks to develop and nurture its diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas and enriches campus life.

Purdue University views, evaluates and treats all persons in any university-related activity or circumstance in which they may be involved solely as individuals on the basis of their own personal abilities, qualifications and other relevant characteristics.

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Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
http://www.purdue.edu/studentregulations/equal_opportunity/studentgrievance.html
https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

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X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
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Course Information
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MW: WTHR 214 (Wetherill Lab of Chemistry)
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Course Description

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Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
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*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

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*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

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*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
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(5) Use of computers in class is limited to assigned work related to class; no use of social networks; no use of internet other than required for class.

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A+	97%-100%	4.33/4.00
A	93%-96%	4.00/4.00
A-	90%-92%	3.67/4.00
B+	87%-89%	3.33/4.00
B	83%-86%	3.00/4.00
B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

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Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
http://www.purdue.edu/studentregulations/equal_opportunity/studentgrievance.html
https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

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Please refer to Purdue's nondiscrimination statement:
http://www.purdue.edu/purdue/ea_eou_statement.html

Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
Two individual assignments *include independent data collection for at least two different crystalline materials. This will be done outside of scheduled class times. Students are required to arrange for use of instruments not later than halfway through the semester, after the student has passed the Online X-ray Safety Training and Quiz for Analytical X-ray Equipment. The origin of the material can be with the student, or a sample can be provided. Where possible, the materials (molecular organic and metal organic compounds, metallic or ceramic solid state materials) will be matched to the research background of the student. Ideally, the material's structure should be unknown and not yet reported. The assignment will involve crystal selection, data collection and processing, structure solution, refinement and validation. The final report should consist of the cif and res file. The exact grade fraction of each assignment will depend on the number and complexity of the individual assignments given out.*

Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
Take home assignment 12, Individual Lab Assignment 2	*200*
Total (40% of total grade)	*1265*

Midterm. 20%
*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

Lab-Practical: 20%
*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

Final. 20%
*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
The ultimate goal of this class is for students to be able to independently use the learned material for analysis of their own samples relating to their research. This part, while necessarily less reflected in the overall grade, relies heavily on engaged participation in the lab section of the class.

Policies

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Purdue University does not condone and will not tolerate Discrimination against any individual on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, disability, status as a veteran, marital status, parental status, sexual orientation, gender identity or gender expression. Purdue University promulgates policies and programs to ensure that all persons have equal access to its employment opportunities and educational programs, services and activities. The principal objective of this policy is to provide fair and consistent treatment for all students and employees of the University. Purdue is committed to increasing the recruitment, selection and promotion of faculty and staff at the University who are racial or ethnic minorities, women, persons with disabilities and veterans. The University also is committed to policies and programs that increase the diversity of the student body.

Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
http://www.purdue.edu/studentregulations/equal_opportunity/studentgrievance.html
https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

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Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
Two individual assignments *include independent data collection for at least two different crystalline materials. This will be done outside of scheduled class times. Students are required to arrange for use of instruments not later than halfway through the semester, after the student has passed the Online X-ray Safety Training and Quiz for Analytical X-ray Equipment. The origin of the material can be with the student, or a sample can be provided. Where possible, the materials (molecular organic and metal organic compounds, metallic or ceramic solid state materials) will be matched to the research background of the student. Ideally, the material's structure should be unknown and not yet reported. The assignment will involve crystal selection, data collection and processing, structure solution, refinement and validation. The final report should consist of the cif and res file. The exact grade fraction of each assignment will depend on the number and complexity of the individual assignments given out.*

Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
Take home assignment 12, Individual Lab Assignment 2	*200*
Total (40% of total grade)	*1265*

Midterm. 20%
*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

Lab-Practical: 20%
*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

Final. 20%
*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
The ultimate goal of this class is for students to be able to independently use the learned material for analysis of their own samples relating to their research. This part, while necessarily less reflected in the overall grade, relies heavily on engaged participation in the lab section of the class.

Policies

General Course Policies

(1) Students are welcome to ask questions outside of class and lecture times, either in person or via e-mail. Phone or text inquiries are likely to be missed or ignored.
(2) Students are encouraged to hand in assignments two or three days early for a first evaluation and suggestions/pointers for improvements. Assignments handed in on the due day will be graded "as received".
(3) Class starts on time. If you are late or have to leave early do so quietly without interrupting others.
(4) Absolutely no cell phone use in class at any time; cell phones have to "remain dark and silent" during the entire class period.
(5) Use of computers in class is limited to assigned work related to class; no use of social networks; no use of internet other than required for class.

Grading

A+	97%-100%	4.33/4.00
A	93%-96%	4.00/4.00
A-	90%-92%	3.67/4.00
B+	87%-89%	3.33/4.00
B	83%-86%	3.00/4.00
B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

Academic Dishonesty

Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Part 5, Section III-B-2-a, Student Regulations] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15, 1972]

***Plagiarism**, in the context of this class, includes **use of ANY material without citation of the original source**. Exceptions are solely material from the assigned text books, and material handed out in class. Sources that should be cited are, but are not limited to, peer reviewed publications, books, non-peer reviewed publications, online*

sources, technical and procedural manuals, and personal communications from others. Use of incorrect material, even if publicly accessible, does not qualify as waiver for wrongly answered questions (exception: peer reviewed indexed publications).

Please also refer to Purdue's student guide for academic integrity:
https://www.purdue.edu/odos/academic-integrity/

Use of Copyrighted Materials
Students are expected, within the context of the Regulations Governing Student Conduct and other applicable University policies, to act responsibly and ethically by applying the appropriate exception under the Copyright Act to the use of copyrighted works in their activities and studies. The University does not assume legal responsibility for violations of copyright law by students who are not employees of the University.

A Copyrightable Work created by any person subject to this policy primarily to express and preserve scholarship as evidence of academic advancement or academic accomplishment. Such works may include, but are not limited to, scholarly publications, journal articles, research bulletins, monographs, books, plays, poems, musical compositions and other works of artistic imagination, and works of students created in the course of their education, such as exams, projects, theses or dissertations, papers and articles.

Please also refer to the University Regulations on policies:
http://www.purdue.edu/policies/academic-research-affairs/ia3.html

Attendance
Students are expected to be present for every meeting of the class. Regular attendance is essential for successfully completing this course. However, no attendance will be taken and excuses will only be required for the dates of mid-term, lab practical and final. Students are required to independently make up missed course sections, and to inquire about assignments if they miss a lecture or lab. When conflicts or absences can be anticipated for the dates of mid-term, lab practical and final, such as for University sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible so that possibly a different date can be scheduled for the test. For unanticipated or emergency absences when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, or by contacting the main chemistry office. When the student is unable to make direct contact with the instructor and is unable to leave word with the department because of circumstances beyond the student's control, and in cases of bereavement, the student or the student's representative should contact the Office of the Dean of Students.

The link to the Purdue's complete policy and implications can be found at:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Missed or Late Work
Homework assignments handed in late will not be accepted (exception: unanticipated or emergency absences, see "Attendance", above). An assignment handed in after the due day 5 pm will incur a zero-point grade.

If a student misses a take home assignment, mid-term, lab practical or final due to unanticipated or emergency absences (see "Attendance", above) a make-up date can be scheduled at the earliest possible date. Unexcused absences incur a zero-point grade.

Grief Absence Policy for Students
Below is the University's Grief Absence Policy for Students:

Purdue University recognizes that a time of bereavement is very difficult for a student. The University therefore provides the following rights to students facing the loss of a family member through the Grief Absence Policy for Students (GAPS). GAPS Policy: Students will be excused for funeral leave and given the opportunity to earn equivalent credit and to demonstrate evidence of meeting the learning outcomes for missed assignments or assessments in the event of the death of a member of the student's family.

See the University's website for additional information:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Violent Behavior Policy
Below is Purdue's policy prohibiting violent behavior:

Purdue University is committed to providing a safe and secure campus environment for members of the university community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent Behavior impedes such goals. Therefore, Violent Behavior is prohibited in or on any University Facility or while participating in any university activity.

See the University's website for additional information:
http://www.purdue.edu/policies/facilities-safety/iva3.html

Mental Health Syllabus Statement

· On the recommendation of the University Senate, CAPS and the Dean the following resources are included in the syllabus.

- **If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack,**

https://purdue.welltrack.com/. Sign in and find information and tools at your fingertips, available to you at any time.

- **If you need support and information about options and resources**, please see the Office of the Dean of Students, http://www.purdue.edu/odos, for drop-in hours (M-F, 8 am- 5 pm).
- **If you're struggling and need mental health services**: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and http://www.purdue.edu/caps/ during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

Emergencies

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

See the University's website for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

Students with Disabilities

The course requires the use of optical microscopes, technical equipment that requires standing and visual alignment of samples, and use of computers in class and for homework assignments and tests. If you have a condition that makes it impossible or difficult to do any of the assigned work then please see the instructor to discuss possible solutions, workarounds or assistance. Academic accommodation must be arranged for BY THE STUDENT through Purdue's Disability Resource Center. The instructor cannot make academic accommodations without a DRC accommodation letter.

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: ***drc@purdue.edu*** *or by phone: 765-494-1247." http://www.purdue.edu/drc/faculty/syllabus.html*

Assistance with Making Learning Materials Accessible. *Purdue's new Innovative Learning group website includes:*

- *Information on Universal Design for learning*
- *Includes our Create Accessible Documents webpage:*

- *How-to training videos and step-by-step documents for faculty to train themselves in making their own course documents accessible*
- *Self-check checklists for evaluation of their own formatting work*
- *Request in-person training on formatting documents*
- *Direct link to request Document Formatting Assistance. The team has 10 student workers ready to assist, and all work is completed in the order it is received.*

Diversity & Inclusion

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Disclaimer

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X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
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Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
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Course Description

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The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
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Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

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Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

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Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
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Total (40% of total grade)	*1265*

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*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

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*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

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B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

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A Copyrightable Work created by any person subject to this policy primarily to express and preserve scholarship as evidence of academic advancement or academic accomplishment. Such works may include, but are not limited to, scholarly publications, journal articles, research bulletins, monographs, books, plays, poems, musical compositions and other works of artistic imagination, and works of students created in the course of their education, such as exams, projects, theses or dissertations, papers and articles.

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Assistance with Making Learning Materials Accessible. *Purdue's new Innovative Learning group website includes:*

- *Information on Universal Design for learning*
- *Includes our Create Accessible Documents webpage:*

- *How-to training videos and step-by-step documents for faculty to train themselves in making their own course documents accessible*
- *Self-check checklists for evaluation of their own formatting work*
- *Request in-person training on formatting documents*
- *Direct link to request Document Formatting Assistance. The team has 10 student workers ready to assist, and all work is completed in the order it is received.*

Diversity & Inclusion

Purdue University is committed to maintaining an inclusive community that recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, Purdue University seeks to develop and nurture its diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas and enriches campus life.

Purdue University views, evaluates and treats all persons in any university-related activity or circumstance in which they may be involved solely as individuals on the basis of their own personal abilities, qualifications and other relevant characteristics.

Purdue University does not condone and will not tolerate Discrimination against any individual on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, disability, status as a veteran, marital status, parental status, sexual orientation, gender identity or gender expression. Purdue University promulgates policies and programs to ensure that all persons have equal access to its employment opportunities and educational programs, services and activities. The principal objective of this policy is to provide fair and consistent treatment for all students and employees of the University. Purdue is committed to increasing the recruitment, selection and promotion of faculty and staff at the University who are racial or ethnic minorities, women, persons with disabilities and veterans. The University also is committed to policies and programs that increase the diversity of the student body.

Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
http://www.purdue.edu/studentregulations/equal_opportunity/studentgrievance.html
https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

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Please refer to Purdue's nondiscrimination statement:
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Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
Two individual assignments *include independent data collection for at least two different crystalline materials. This will be done outside of scheduled class times. Students are required to arrange for use of instruments not later than halfway through the semester, after the student has passed the Online X-ray Safety Training and Quiz for Analytical X-ray Equipment. The origin of the material can be with the student, or a sample can be provided. Where possible, the materials (molecular organic and metal organic compounds, metallic or ceramic solid state materials) will be matched to the research background of the student. Ideally, the material's structure should be unknown and not yet reported. The assignment will involve crystal selection, data collection and processing, structure solution, refinement and validation. The final report should consist of the cif and res file. The exact grade fraction of each assignment will depend on the number and complexity of the individual assignments given out.*

Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
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- *How-to training videos and step-by-step documents for faculty to train themselves in making their own course documents accessible*
- *Self-check checklists for evaluation of their own formatting work*
- *Request in-person training on formatting documents*
- *Direct link to request Document Formatting Assistance. The team has 10 student workers ready to assist, and all work is completed in the order it is received.*

Diversity & Inclusion

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Purdue University does not condone and will not tolerate Discrimination against any individual on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, disability, status as a veteran, marital status, parental status, sexual orientation, gender identity or gender expression. Purdue University promulgates policies and programs to ensure that all persons have equal access to its employment opportunities and educational programs, services and activities. The principal objective of this policy is to provide fair and consistent treatment for all students and employees of the University. Purdue is committed to increasing the recruitment, selection and promotion of faculty and staff at the University who are racial or ethnic minorities, women, persons with disabilities and veterans. The University also is committed to policies and programs that increase the diversity of the student body.

Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
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https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

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Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
Two individual assignments *include independent data collection for at least two different crystalline materials. This will be done outside of scheduled class times. Students are required to arrange for use of instruments not later than halfway through the semester, after the student has passed the Online X-ray Safety Training and Quiz for Analytical X-ray Equipment. The origin of the material can be with the student, or a sample can be provided. Where possible, the materials (molecular organic and metal organic compounds, metallic or ceramic solid state materials) will be matched to the research background of the student. Ideally, the material's structure should be unknown and not yet reported. The assignment will involve crystal selection, data collection and processing, structure solution, refinement and validation. The final report should consist of the cif and res file. The exact grade fraction of each assignment will depend on the number and complexity of the individual assignments given out.*

Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
Take home assignment 12, Individual Lab Assignment 2	*200*
Total (40% of total grade)	*1265*

Midterm. 20%
*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

Lab-Practical: 20%
*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

Final. 20%
*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
The ultimate goal of this class is for students to be able to independently use the learned material for analysis of their own samples relating to their research. This part, while necessarily less reflected in the overall grade, relies heavily on engaged participation in the lab section of the class.

Policies

General Course Policies

(1) Students are welcome to ask questions outside of class and lecture times, either in person or via e-mail. Phone or text inquiries are likely to be missed or ignored.
(2) Students are encouraged to hand in assignments two or three days early for a first evaluation and suggestions/pointers for improvements. Assignments handed in on the due day will be graded "as received".
(3) Class starts on time. If you are late or have to leave early do so quietly without interrupting others.
(4) Absolutely no cell phone use in class at any time; cell phones have to "remain dark and silent" during the entire class period.
(5) Use of computers in class is limited to assigned work related to class; no use of social networks; no use of internet other than required for class.

Grading

A+	97%-100%	4.33/4.00
A	93%-96%	4.00/4.00
A-	90%-92%	3.67/4.00
B+	87%-89%	3.33/4.00
B	83%-86%	3.00/4.00
B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

Academic Dishonesty

Purdue prohibits "dishonesty in connection with any University activity. Cheating, plagiarism, or knowingly furnishing false information to the University are examples of dishonesty." [Part 5, Section III-B-2-a, Student Regulations] Furthermore, the University Senate has stipulated that "the commitment of acts of cheating, lying, and deceit in any of their diverse forms (such as the use of substitutes for taking examinations, the use of illegal cribs, plagiarism, and copying during examinations) is dishonest and must not be tolerated. Moreover, knowingly to aid and abet, directly or indirectly, other parties in committing dishonest acts is in itself dishonest." [University Senate Document 72-18, December 15, 1972]

***Plagiarism**, in the context of this class, includes **use of ANY material without citation of the original source**. Exceptions are solely material from the assigned text books, and material handed out in class. Sources that should be cited are, but are not limited to, peer reviewed publications, books, non-peer reviewed publications, online*

sources, technical and procedural manuals, and personal communications from others. Use of incorrect material, even if publicly accessible, does not qualify as waiver for wrongly answered questions (exception: peer reviewed indexed publications).

Please also refer to Purdue's student guide for academic integrity:
https://www.purdue.edu/odos/academic-integrity/

Use of Copyrighted Materials
Students are expected, within the context of the Regulations Governing Student Conduct and other applicable University policies, to act responsibly and ethically by applying the appropriate exception under the Copyright Act to the use of copyrighted works in their activities and studies. The University does not assume legal responsibility for violations of copyright law by students who are not employees of the University.

A Copyrightable Work created by any person subject to this policy primarily to express and preserve scholarship as evidence of academic advancement or academic accomplishment. Such works may include, but are not limited to, scholarly publications, journal articles, research bulletins, monographs, books, plays, poems, musical compositions and other works of artistic imagination, and works of students created in the course of their education, such as exams, projects, theses or dissertations, papers and articles.

Please also refer to the University Regulations on policies:
http://www.purdue.edu/policies/academic-research-affairs/ia3.html

Attendance
Students are expected to be present for every meeting of the class. Regular attendance is essential for successfully completing this course. However, no attendance will be taken and excuses will only be required for the dates of mid-term, lab practical and final. Students are required to independently make up missed course sections, and to inquire about assignments if they miss a lecture or lab. When conflicts or absences can be anticipated for the dates of mid-term, lab practical and final, such as for University sponsored activities and religious observations, the student should inform the instructor of the situation as far in advance as possible so that possibly a different date can be scheduled for the test. For unanticipated or emergency absences when advance notification to an instructor is not possible, the student should contact the instructor as soon as possible by email, or by contacting the main chemistry office. When the student is unable to make direct contact with the instructor and is unable to leave word with the department because of circumstances beyond the student's control, and in cases of bereavement, the student or the student's representative should contact the Office of the Dean of Students.

The link to the Purdue's complete policy and implications can be found at:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Missed or Late Work
Homework assignments handed in late will not be accepted (exception: unanticipated or emergency absences, see "Attendance", above). An assignment handed in after the due day 5 pm will incur a zero-point grade.

If a student misses a take home assignment, mid-term, lab practical or final due to unanticipated or emergency absences (see "Attendance", above) a make-up date can be scheduled at the earliest possible date. Unexcused absences incur a zero-point grade.

Grief Absence Policy for Students
Below is the University's Grief Absence Policy for Students:

Purdue University recognizes that a time of bereavement is very difficult for a student. The University therefore provides the following rights to students facing the loss of a family member through the Grief Absence Policy for Students (GAPS). GAPS Policy: Students will be excused for funeral leave and given the opportunity to earn equivalent credit and to demonstrate evidence of meeting the learning outcomes for missed assignments or assessments in the event of the death of a member of the student's family.

See the University's website for additional information:
http://www.purdue.edu/studentregulations/regulations_procedures/classes.html

Violent Behavior Policy
Below is Purdue's policy prohibiting violent behavior:

Purdue University is committed to providing a safe and secure campus environment for members of the university community. Purdue strives to create an educational environment for students and a work environment for employees that promote educational and career goals. Violent Behavior impedes such goals. Therefore, Violent Behavior is prohibited in or on any University Facility or while participating in any university activity.

See the University's website for additional information:
http://www.purdue.edu/policies/facilities-safety/iva3.html

Mental Health Syllabus Statement

· On the recommendation of the University Senate, CAPS and the Dean the following resources are included in the syllabus.

- **If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack,**

https://purdue.welltrack.com/. Sign in and find information and tools at your fingertips, available to you at any time.

- **If you need support and information about options and resources**, please see the Office of the Dean of Students, http://www.purdue.edu/odos, for drop-in hours (M-F, 8 am- 5 pm).
- **If you're struggling and need mental health services**: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and http://www.purdue.edu/caps/ during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

Emergencies

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

See the University's website for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

Students with Disabilities

The course requires the use of optical microscopes, technical equipment that requires standing and visual alignment of samples, and use of computers in class and for homework assignments and tests. If you have a condition that makes it impossible or difficult to do any of the assigned work then please see the instructor to discuss possible solutions, workarounds or assistance. Academic accommodation must be arranged for BY THE STUDENT through Purdue's Disability Resource Center. The instructor cannot make academic accommodations without a DRC accommodation letter.

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: ***drc@purdue.edu*** *or by phone: 765-494-1247." http://www.purdue.edu/drc/faculty/syllabus.html*

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Disclaimer

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X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
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Course Description

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The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
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Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

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Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
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Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
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Take home assignments - breakdown and points:

Take home assignment 1, Miller indices and Bragg Planes	*50*
Take home assignment 2, Symmetry	*75*
Take home assignment 3, Space Groups	*50*
Take home assignment 4, Structure refinement 1 – Mid sized molecule 1	*75*
Take home assignment 5, Structure refinement 2 – Mid sized molecule 2	*75*
Take home assignment 6, Structure refinement 3 – Simple disorder	*75*
Take home assignment 7, Structure refinement 4 – Multiple Disorder	*75*
Take home assignment 8, Structure Evaluation	*150*
Take home assignment 9, Prep for Finals 1	*120*
Take home assignment 10, Prep for Finals 2	*120*
Take home assignment 11, Individual Lab Assignment 1	*200*
Take home assignment 12, Individual Lab Assignment 2	*200*
Total (40% of total grade)	*1265*

Midterm. 20%
*Date about halfway through the semester, **tentatively March 4th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

Lab-Practical: 20%
*An open book exam. It will be held about two thirds into the semester during one three-hour period. **Tentatively April 22nd** (subject to room availability). Students are expected to demonstrate that they are able to independently solve and refine a moderately complicated molecular solid state structure from single crystal data.*

Final. 20%
*During Finals week, **tentatively May 6th** (subject to room availability). Open book exam, 2hrs. Focus is on understanding of material covered in class and in previous assignments.*

How to Succeed in This Course

*Most important for succeeding in this class is **active participation**, and careful and thorough work on take home assignments and exercises. The assignments and exercises provide the opportunity for in depth analysis of class material beyond what can be picked up during lecture. The focus is on understanding and comprehension. There will be no solely multiple choice based tests.*
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A	93%-96%	4.00/4.00
A-	90%-92%	3.67/4.00
B+	87%-89%	3.33/4.00
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B-	80%-82%	2.67/4.00
C+	77%-79%	2.33/4.00
C	73%-76%	2.00/4.00
C-	70%-72%	1.67/4.00
D+	67%-69%	1.33/4.00
D	63%-66%	1.00/4.00
D-	60%-62%	0.67/4.00
F	0%-59%	0.00/4.00

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A Copyrightable Work created by any person subject to this policy primarily to express and preserve scholarship as evidence of academic advancement or academic accomplishment. Such works may include, but are not limited to, scholarly publications, journal articles, research bulletins, monographs, books, plays, poems, musical compositions and other works of artistic imagination, and works of students created in the course of their education, such as exams, projects, theses or dissertations, papers and articles.

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Mental Health Syllabus Statement

· On the recommendation of the University Senate, CAPS and the Dean the following resources are included in the syllabus.

- **If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try WellTrack,**

https://purdue.welltrack.com/. Sign in and find information and tools at your fingertips, available to you at any time.

- **If you need support and information about options and resources**, please see the Office of the Dean of Students, http://www.purdue.edu/odos, for drop-in hours (M-F, 8 am- 5 pm).
- **If you're struggling and need mental health services**: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and http://www.purdue.edu/caps/ during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

Emergencies

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

See the University's website for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

Students with Disabilities

The course requires the use of optical microscopes, technical equipment that requires standing and visual alignment of samples, and use of computers in class and for homework assignments and tests. If you have a condition that makes it impossible or difficult to do any of the assigned work then please see the instructor to discuss possible solutions, workarounds or assistance. Academic accommodation must be arranged for BY THE STUDENT through Purdue's Disability Resource Center. The instructor cannot make academic accommodations without a DRC accommodation letter.

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: ***drc@purdue.edu*** *or by phone: 765-494-1247." http://www.purdue.edu/drc/faculty/syllabus.html*

Assistance with Making Learning Materials Accessible. *Purdue's new Innovative Learning group website includes:*

- *Information on Universal Design for learning*
- *Includes our Create Accessible Documents webpage:*

- *How-to training videos and step-by-step documents for faculty to train themselves in making their own course documents accessible*
- *Self-check checklists for evaluation of their own formatting work*
- *Request in-person training on formatting documents*
- *Direct link to request Document Formatting Assistance. The team has 10 student workers ready to assist, and all work is completed in the order it is received.*

Diversity & Inclusion

Purdue University is committed to maintaining an inclusive community that recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, Purdue University seeks to develop and nurture its diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas and enriches campus life.

Purdue University views, evaluates and treats all persons in any university-related activity or circumstance in which they may be involved solely as individuals on the basis of their own personal abilities, qualifications and other relevant characteristics.

Purdue University does not condone and will not tolerate Discrimination against any individual on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, disability, status as a veteran, marital status, parental status, sexual orientation, gender identity or gender expression. Purdue University promulgates policies and programs to ensure that all persons have equal access to its employment opportunities and educational programs, services and activities. The principal objective of this policy is to provide fair and consistent treatment for all students and employees of the University. Purdue is committed to increasing the recruitment, selection and promotion of faculty and staff at the University who are racial or ethnic minorities, women, persons with disabilities and veterans. The University also is committed to policies and programs that increase the diversity of the student body.

Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
http://www.purdue.edu/studentregulations/equal_opportunity/studentgrievance.html
https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

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excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life.

Purdue University prohibits discrimination against any member of the University community on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, marital status, parental status, sexual orientation, gender identity and expression, disability, or status as a veteran. The University will conduct its programs, services and activities consistent with applicable federal, state and local laws, regulations and orders and in conformance with the procedures and limitations as set forth in Executive Memorandum No. D-1, which provides specific contractual rights and remedies. Any student who believes they have been discriminated against may visit www.purdue.edu/report-hate to submit a complaint to the Office of Institutional Equity. Information may be reported anonymously.

Please refer to Purdue's nondiscrimination statement:
http://www.purdue.edu/purdue/ea_eou_statement.html

Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.

X-ray Crystallography 12650 - CHM 69600-006

Dr. Matthias Zeller
Office: WTHR 101
Phone: 765-494-4572 (office)
Email: zeller4@purdue.edu
Office Hours: Mon-Fri, 9 am – 5 pm
www.chem.purdue.edu/xray/

Course Information
Spring, 2020
MWF, 3:30-4:20 pm
MW: WTHR 214 (Wetherill Lab of Chemistry)
3 Course Credit Hours or audit (1 Course Credit)
https://www.chem.purdue.edu/xray/Class.php

Course Description

The course will introduce you to X-ray crystallography and X-ray diffraction, the only widely used techniques for determination of accurate structural data at the atomic and molecular level. The main goal of the class is to prepare you to independently use this and related techniques as an analysis tool for your own research in fields such as synthetic and analytic organic and inorganic chemistry, metal-organic materials and frameworks, materials science, pharmaceutical sciences, geochemistry, and others; and to enable you to evaluate the work of others.
The course is divided in two sections: A lecture section focusing on the basics and theory of X-ray crystallography and X-ray diffraction; and a hands-on laboratory section which aims to prepare you to be able to independently deploy the technique for own use. Some aspects of other diffraction techniques will be covered (powder and multicrystalline XRD, extended solids (metals, ceramics), macromolecular XRD), but the main focus of this course is on structural analysis of small molecule crystalline materials.
The class will be held in either a lecture hall / computer lab (Wetherill Laboratory of Chemistry 214), or in the X-ray Diffraction Laboratory (Wetherill 101). In the hands-on lab section students will learn to use modern X-ray diffractometers and diffraction software. We will use the chemistry departments two new top of the line single crystal diffractometers (installed Dec 2016), starting with selection, mounting and evaluation of crystals to full analysis and evaluation of the resultant crystal structures. Collection and analysis of data will make use of the Bruker Apex3 program suite. Data will be refined and analyzed using XPREP, Shelxl, Shelxtl, Shelxle, Platon, and verified using the checkcif procedure. Various data bases are available to assist in data analysis and refinement.
Students are encouraged to "bring their own crystals" for analysis during the course.

Prerequisites

This is a graduate level course.
Basic knowledge of some or all of the following is helpful, but no in depth knowledge of all topics is required. Please consult with the instructor if you are not sure if you have all the prerequisites for this course.

Basic math skills (matrix calculation, vector geometry, real and imaginary numbers). Basic optics (the nature of waves, electromagnetic radiation, the electromagnetic spectrum). The nature of the atom. The nature of chemical bonding (covalent, metallic and ionic bonding, van der Waals interactions, hydrogen bonding). General, organic and inorganic chemistry (some advanced courses). Some solid state chemistry (cubic and hexagonal dense packing). Physical chemistry (solubility, phase equilibria, IR and Raman spectroscopy, zero point vibration, molecular symmetry as used in spectroscopy, character tables). Chemical ethics.

Learning Outcomes

- *Basics and theoretical concepts of X-ray diffraction.*
- *Knowledge of the process of crystal structure analysis.*
- *Types of instrumentation, hardware and technology used in X-ray diffraction.*
- *Independent collection of single crystal XRD data. Evaluation of crystals, diffraction data and their suitability for single crystal structure analysis.*
- *Independent workup and reduction of raw diffraction data. Solving and refinement of crystal data up to refinement of simple disorder.*
- *Learning to make "the right choices for my experiment".*

Required Texts

Class handouts and notes cover all required material and there are no specific text books for this class. For further reading and study the following texts are suggested:

Crystal Structure Analysis, Principle and Practice (International Union of Crystallography Monographs on Crystallography 13), Blake, Clegg, Cole, Evans, Main, Parsons, Watkin, Editor William Clegg.
***ISBN**: 9780199219469*

Crystal Structure Refinement: A Crystallographer's Guide to SHELXL (International Union of Crystallography Monographs on Crystallography) Peter Müller, Regine Herbst-Irmer, Anthony L. Spek, Thomas Schneider, and Michael Sawaya.
***ISBN**: 9780198570769*

Course Requirements

The following is an outline of the structure of the class and fractions of grades assigned to each section in percent of the total grade. The class is open for audit (no grade assigned).

***Online X-ray Safety Training and Quiz for Analytical X-ray Equipment: 0%**,*

Students must pass to take part in the independent parts of the laboratory section and be permitted to operate the lab equipment,
https://www.purdue.edu/ehps/rem/home/training.htm#rs

Homework assignments and take home exams. 40%
Twelve take home assignments will be given throughout the semester on a variety of topics. The assignments will focus on both theory and background (lecture section of the course) as well as practice (lab section of the course). All take home assignments are open book. Discussion among students is encouraged, but all handed in work has to be the work of each individual student. All material used has to be properly referenced and scientific ethics rules have to be strictly followed (the same rules as for scientific peer reviewed publications apply).

Lecture section: There will be ***six graded take home assignments*** *focused on Background and theory assignments (three in January, and two prior to Finals). These assignments will focus more on understanding and comprehension than an ability to repeat course material. For background and theory assignments there will often not be a "correct answer", but the students will have to discuss a topic to show that they have an in-depth understanding of the material. Some assignments will require independent research into topics not fully covered in the lecture part of the course.*

Lab section: There will be ***six graded take home assignments*** *that focus on collection, processing and refinement of single crystal structure data.* ***Four common assignments*** *given to all students will include solution and refinement of several single crystal datasets, which will parallel similar work done in the lab section of the class. The results (res and cif files) will be graded for correctness and completeness. Additional practice data sets are provided for students. Data sets are sorted by level of complexity and follow that of the examples used in class and for take home assignments. Solving and refining of at least some of the practice data sets is highly encouraged, but not required.*
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D	63%-66%	1.00/4.00
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https://purdue.welltrack.com/. Sign in and find information and tools at your fingertips, available to you at any time.

- **If you need support and information about options and resources**, please see the Office of the Dean of Students, http://www.purdue.edu/odos, for drop-in hours (M-F, 8 am- 5 pm).
- **If you're struggling and need mental health services**: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact Counseling and Psychological Services (CAPS) at (765)494-6995 and http://www.purdue.edu/caps/ during and after hours, on weekends and holidays, or by going to the CAPS office of the second floor of the Purdue University Student Health Center (PUSH) during business hours.

Emergencies

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.

See the University's website for additional information:
https://www.purdue.edu/ehps/emergency_preparedness/

Students with Disabilities

The course requires the use of optical microscopes, technical equipment that requires standing and visual alignment of samples, and use of computers in class and for homework assignments and tests. If you have a condition that makes it impossible or difficult to do any of the assigned work then please see the instructor to discuss possible solutions, workarounds or assistance. Academic accommodation must be arranged for BY THE STUDENT through Purdue's Disability Resource Center. The instructor cannot make academic accommodations without a DRC accommodation letter.

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: ***drc@purdue.edu*** *or by phone: 765-494-1247." http://www.purdue.edu/drc/faculty/syllabus.html*

Assistance with Making Learning Materials Accessible. *Purdue's new Innovative Learning group website includes:*

- *Information on Universal Design for learning*
- *Includes our Create Accessible Documents webpage:*

- *How-to training videos and step-by-step documents for faculty to train themselves in making their own course documents accessible*
- *Self-check checklists for evaluation of their own formatting work*
- *Request in-person training on formatting documents*
- *Direct link to request Document Formatting Assistance. The team has 10 student workers ready to assist, and all work is completed in the order it is received.*

Diversity & Inclusion

Purdue University is committed to maintaining an inclusive community that recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic excellence, Purdue University seeks to develop and nurture its diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas and enriches campus life.

Purdue University views, evaluates and treats all persons in any university-related activity or circumstance in which they may be involved solely as individuals on the basis of their own personal abilities, qualifications and other relevant characteristics.

Purdue University does not condone and will not tolerate Discrimination against any individual on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, disability, status as a veteran, marital status, parental status, sexual orientation, gender identity or gender expression. Purdue University promulgates policies and programs to ensure that all persons have equal access to its employment opportunities and educational programs, services and activities. The principal objective of this policy is to provide fair and consistent treatment for all students and employees of the University. Purdue is committed to increasing the recruitment, selection and promotion of faculty and staff at the University who are racial or ethnic minorities, women, persons with disabilities and veterans. The University also is committed to policies and programs that increase the diversity of the student body.

Here are some links that may be relevant:
http://www.purdue.edu/policies/ethics/iiic2.html
http://www.purdue.edu/studentregulations/equal_opportunity/studentgrievance.html
https://www.purdue.edu/studentsuccess/specialized/drc/faculty/index.html

Nondiscrimination

Purdue University is committed to maintaining a community which recognizes and values the inherent worth and dignity of every person; fosters tolerance, sensitivity, understanding, and mutual respect among its members; and encourages each individual to strive to reach his or her own potential. In pursuit of its goal of academic

excellence, the University seeks to develop and nurture diversity. The University believes that diversity among its many members strengthens the institution, stimulates creativity, promotes the exchange of ideas, and enriches campus life.

Purdue University prohibits discrimination against any member of the University community on the basis of race, religion, color, sex, age, national origin or ancestry, genetic information, marital status, parental status, sexual orientation, gender identity and expression, disability, or status as a veteran. The University will conduct its programs, services and activities consistent with applicable federal, state and local laws, regulations and orders and in conformance with the procedures and limitations as set forth in Executive Memorandum No. D-1, which provides specific contractual rights and remedies. Any student who believes they have been discriminated against may visit www.purdue.edu/report-hate to submit a complaint to the Office of Institutional Equity. Information may be reported anonymously.

Please refer to Purdue's nondiscrimination statement:
http://www.purdue.edu/purdue/ea_eou_statement.html

Class Schedule

***Midterm**, **tentatively March 4th** (subject to room availability).*
***Lab-Practical, tentatively April 22nd** (subject to room availability).*
***Final**, **tentatively May 6th** (subject to room availability).*

Topics that will be covered in mid terms and finals will be announced ca. two weeks ahead of the scheduled dates and generally include all topics covered until the scheduled date of the test.

Dates for readings, assignments, labs, etc, will be announced as class proceeds.

Disclaimer

This syllabus is subject to change.