General Information:

Instructor: Cora Lind-Kovacs
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Phone: (419) 530-1505
e-mail: cora.lind@utoledo.edu

Classes: MW 8:00-9:40, BO 2850

Office Hours: MTWR 10-11, or by appointment

Help: Please do not hesitate to stop by to ask questions during Office Hours! If you cannot make any of the normal Office Hours, you can set up an appointment at other times by phone or e-mail. Please do set up an appointment instead of randomly stopping by – this will assure that I have time for you, and allow me to focus on other things when necessary!

Text(s): Class handouts can be downloaded from http://homepages.utoledo.edu/clind. These should be considered as an outline of the lectures that will save you from having to copy complicated drawings. You should augment them with your own notes during class. It is not necessary to buy a text book for this class, although you are encouraged to buy some crystallography book you like if you plan on using crystallography in your research. One of the cheapest and most comprehensive options I have found is “Structure Determination by X-ray Crystallography”, by Ladd and Palmer. Parts of the “International Tables for Crystallography, Vol. A” will also be used in class (copies of necessary pages will be provided). These textbooks aid in following the class and getting additional problems or views on topics. For Ladd and Palmer it does not matter whether you get the 5th or an older edition. If your research deals with crystallography, it is highly recommended that you invest in a crystallography textbook at some point in time. Both of these books, and some other crystallography text books, are available in WO 2262 and in the library. For my books in WO 2262, there will be a 2 h time limit for taking them to a different room, and you must sign your name and room number on the white board.

Grading: The course grade will be based on the following:
- Homework (5 sets, 3% each) 15%
- Projects (Best 2 out of 3, 10% each) 20%
- 2 in-class exams (20% each) 40%
- Final exam 25%
- IYCr2014 extra credit opportunity 3%

If you score 85% or higher on the final comprehensive exam, your worst grade (combined homework grade, individual project grade, individual in-class exam grade) will be dropped for the final grade calculation. Final grades are based on a simple 5% interval scale, and you need to earn the following minimum percentages to achieve the corresponding grades: 90% A, 85% A-, 80% B+, 75% B, 70% B-, 65% C+, 60% C, 55% C-, 50% D+, 45% D, 40% D-. Please note that grades will NOT be curved, so you can calculate where you stand at any time!
**Five homework assignments** will be given in class at least one week before the work is due. Assignments are due at the beginning of class. If there are special circumstances that necessitate that you hand your homework in late (e.g., 3 exams that week, medical issues in the family, conference attendance etc.), please inform me ASAP so that we can negotiate a different due date. You may work on homework in groups, however, it is recommended that you make sure you understand the problem solving process and do not simply copy someone else’s results! Start your homework early - some of the problems can be challenging, but this is the place where you can actually review what you learned in class and figure out what it means and how to apply it. And yes, please do feel free to stop by during office hours to get help with the homework – this is not just possible, but actually strongly recommended if you get stuck on something!

**Three projects** will be assigned as the class proceeds, one on indexing, one on single crystal structure solution, and one on Rietveld refinement. An appropriate introduction to the theories and programs necessary to complete the projects will be given before the projects are assigned. I assume that you have a laptop that you can use for these projects – *if you do not own a laptop please inform me ASAP so that I can try to negotiate with the department about borrowing computers for the class periods designated to the projects!* Projects will be due in class one to two weeks after the initial assignment date. The grades of **two projects** will be included in your final grade. If you hand in all three projects, the two best grades will be counted. If you choose to hand in only two projects, those two grades will count towards your final grade.

The **two in-class exams** will be given during class periods on

**Wednesday, 10/1 and Wednesday, 11/5**

The **final exam** will take place during the scheduled time on

**Monday, 12/15 (8-10 am)**

Make-up exams will only be given for excused absences (refer to the “University of Toledo Missed Class Policy” for excused absence situations).

**No classes** will be held on 9/1 (Labor Day), 10/13 (Fall Break), and 11/26 (Thanksgiving Break).

2014 has been designated as “International Year of Crystallography” by UNESCO. Stay tuned for a variety of opportunities to participate in outreach to bring crystallography/crystal growing to local schools or scout groups, or to help prepare handouts for teachers. You are not required to participate in any of these activities, but if you do, you will receive a 3% “IYCr2014 extra credit” bonus towards your class grade!

**Course description:**
This course has no prerequisites, however, some math background (integration, vector algebra, sine/cosine/exp functions) is expected. A brief recap of math rules used for problem solving and deriving equations will be given in class. If you would like more review on math, please stop by during office hours, and I will be glad to help you with it!

The course is concerned with the basic principles governing X-ray crystallography. This will include a detailed treatment of crystal symmetry, point, plane and space groups, as well as a physical/mathematical treatment of the laws of diffraction. Reciprocal space concepts will be used to facilitate the understanding of diffraction experiments (don’t worry if this does not yet mean anything to you – it will by the end of the course!). Methods of data collection, treatment and interpretation will be covered, and you will be able to get some hands-on experience in data treatment with three class projects. At the end of the class, you should have acquired a thorough understanding of crystal symmetry and standard diffraction methods. This will allow you to collect and interpret your own data for simple cases, and will give you
the necessary background to tackle more difficult problems with some experts’ help. The knowledge will also be beneficial for reading, interpreting and critically evaluating crystallography related papers.

**Course policies:**
Class attendance is strongly recommended. The textbook assigned for this class is a very useful tool, however, lectures will cover some topics that are not detailed in the book. You will be responsible for the material covered in all classes (and homework assignments and projects), whether you attend them or not. Asking questions during class is strongly encouraged. Please do not be afraid to speak up if you are unclear about something! There are probably several other students who are having trouble with the same point, and it will allow me to clarify the topic for you.

You can drop this class with no record on your transcript until 9/8. Withdrawal between 9/8 and 10/31S will result in a ‘W’ grade. You cannot drop the course after 10/31.

Academic dishonesty as outlined in the University of Toledo policies will not be tolerated and may result in an ‘F’ grade for the class.

**Resources for crystallography:**
**Course texts:**

**Other books:**
   - A good book that covers physical/mathematical backgrounds of diffraction and applications.
   - A simpler version of book 3).
   - A good introductory book.
   - A good crystallography book, but not for absolute beginners.
   - A classic. Very mathematical/abstract. This book is about X-ray scattering not crystal structure determination.
   - Primarily about powder methods.
   - The only book devoted to Rietveld analysis (the last step in the extraction of structural information from powder data).
   - The first comprehensive book about all steps involved in structure determination from powder data.

**Web pages:**
- [http://www.hwi.buffalo.edu/ACA/](http://www.hwi.buffalo.edu/ACA/) (American Crystallographic Association)
- [http://www.ccp14.ac.uk/](http://www.ccp14.ac.uk/) (CCP14 home page, good source for crystallographic programs)

These web pages also provide extensive resource lists and links to other web pages.
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<td>August 25-29</td>
<td>Introduction Crystals</td>
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<td>2</td>
<td>September 1-5</td>
<td><strong>LABOR DAY</strong> Symmetry Point and space groups</td>
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<td>3</td>
<td>September 8-12</td>
<td>Plane and space groups Symmetry exercises</td>
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<td>4</td>
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<td>Diffraction Reciprocal space</td>
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<td>5</td>
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<td>Reciprocal space Structure Factors</td>
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| 6    | September 29-October 3 | Review  
|      |                 | EXAM I on 10/1                                             |
| 7    | October 6-10    | Fourier Transforms Data collection                         |
| 8    | October 13-17   | **FALL BREAK** Structure solution: Patterson maps          |
| 9    | October 20-24   | Structure solution: Fourier maps, MIR, MAD Project I: Indexing of powder patterns |
| 10   | October 27-31   | Project I (hands-on)                                       |
| 11   | November 3-7    | Review EXAM II on 11/5                                     |
| 12   | November 10-14  | Structure refinement Structure interpretation Synchrotrons and Neutrons |
| 13   | November 17-21  | Project II: Solving a single crystal structure (Kristin Kirschbaum, IC) |
| 14   | November 24-28  | Project II: Solving a single crystal structure **Thanksgiving** |
| 15   | December 1-5    | Project III: Rietveld refinement (lecture+hands-on)         |
| 16   | December 8-12   | Project III Review                                         |
| 17   | December 15-19  | **FINAL EXAM on 12/15**                                    |