INSTRUCTOR: Dr. Alan J. Jircitano
OFFICE: 33 Hammermill
PHONE: 898-6400
INTERNET: jircitano@psu.edu
http://chemistry.bd.psu.edu/jircitano/
OFFICE HOURS: M 9 - 10, T 11 - 12, F 10 - 11 and by appointment
TEXT: PowerPoint Notes
Principles of X-ray Crystallography – Li-ling Ooi

COURSE CONTENT:

Introduction
CIF
Crystals
  Growth
  Selection
  Properties
  Sample Preparation
Diffraction of X-rays
  X-ray Sources
  Lattices, Planes, and Indices
  Bragg's Law
  Reciprocal Space
Symmetry Operations and Space Groups
Data Collection
  Geometric
  Intensity
  Diffractometers and Computers
Data Reduction
Structure Factors and Fourier Synthesis
The Phase Problem
  Heavy Atom Method: Patterson Maps and Harker Lines and Planes
  Direct Methods
Refinement
Derived Results
Computer Programs
  Structured Solution Software: SHELXS and SHELXL
  Graphics: ORTEP
A Real Crystal Structure
Publication - CIF format
EXAMS:

There will be two (2) 100 point take home exams. Daily problems (along with class participation) are worth a total of 100 points. The final (also take home) will consist of answering questions based on a current journal article of a crystal structure and is worth 100 points. The class total is 400 points.

GRADING:

<table>
<thead>
<tr>
<th>Grade</th>
<th>Range</th>
<th>Grade</th>
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</thead>
<tbody>
<tr>
<td>A</td>
<td>100 - 93%</td>
<td>C+</td>
<td>77 - 79%</td>
</tr>
<tr>
<td>A−</td>
<td>90 - 92%</td>
<td>C</td>
<td>70 - 76%</td>
</tr>
<tr>
<td>B+</td>
<td>87 - 89%</td>
<td>D</td>
<td>60 - 69%</td>
</tr>
<tr>
<td>B</td>
<td>83 - 86%</td>
<td>F</td>
<td>0 - 59%</td>
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<tr>
<td>B−</td>
<td>80 - 82%</td>
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Your final grade will be influenced by such factors as attendance and class participation.

POLICIES:

1. If you find yourself lost or confused at any time, see me after class. The material is very cumulative. Do not wait until the last week to ask questions.

2. Class attendance is expected.

Academic Integrity

Academic integrity is a basic guiding principle for all academic activity at the University, and all members of the community are expected to adhere to this principle. Specifically, academic integrity is the pursuit of scholarly activity in an open, honest, and responsible manner. It includes a commitment not to engage in or tolerate acts of falsification, misrepresentation, or deception. Such acts violate the fundamental ethical principles of the University community and undermine the efforts of others.

Violations of academic integrity are not tolerated at Penn State Behrend. Violators will receive academic sanctions and may receive disciplinary sanctions, including the awarding of an XF grade. In cases such as these, an XF grade is recorded on the transcript and states that failure of the course was due to an act of academic dishonesty. All acts of academic dishonesty are recorded so those repeat offenders can be sanctioned accordingly.

For more information: http://behrend.psu.edu/for-faculty-staff/faculty-resources/academic-integrity
Disabilities and Learning Differences

Penn State is strongly committed to providing full access to its programs and services for all individuals. The University encourages academically qualified students with disabilities to take advantage of the educational programs and accommodations offered at Penn State Behrend.


Educational Equity Concerns

Penn State takes great pride to foster a diverse and inclusive environment for students, faculty, and staff. Acts of intolerance, discrimination, harassment, and/or incivility due to age, ancestry, color, disability, gender, national origin, race, religious belief, sexual orientation, or veteran status are not tolerated and can be reported through Educational Equity at the Report Bias site: [http://equity.psu.edu/reportbias/statement](http://equity.psu.edu/reportbias/statement).

Counseling and Psychological Services

Students with academic concerns related to this course should contact the instructor in person or via email. Students also may occasionally have personal issues that arise in the course of pursuing higher education that may interfere with their academic performance. If you find yourself facing problems affecting your coursework, you are encouraged to talk with an instructor and to seek confidential assistance at the Penn State Behrend Personal Counseling Services at (814) 898-6504.

For more information: [http://psbehrend.psu.edu/student-life/student-services/personal-counseling](http://psbehrend.psu.edu/student-life/student-services/personal-counseling)

Tutoring Help:

Contact the Learning Resource Center (LRC) at [http://behrend.psu.edu/tutorappointments](http://behrend.psu.edu/tutorappointments) to make an appointment.

Special Note:

Do you receive loans, grants, or work study to help pay for college? Every semester Penn State is required by law to review your academic progress and determine your eligibility for financial aid for the future term. There are three components to making satisfactory academic progress: degree status, completion rate of attempted credits, and time-to-degree limits.

Degree status: If you are dropped from degree status, which may occur if you do not maintain a C average, you are ineligible for state and federal student aid - including loans.
Completion rate of attempted credits: You must earn a minimum of 67% of your cumulative attempted credits.
Time-to-degree: If you exceed 150 percent of the number of credits required for your degree
program, you will have exceeded the time-to-degree limit. Work with your academic advisor to make sure you finish your degree in four years.

Questions about how your academic actions can affect your financial aid?
Financial Aid Office, 2nd floor of the Metzgar Center
814-898-6162
behrendfinaid@psu.edu
https://studentaid.psu.edu/eligibility/satisfactory-academic-progress