INSTRUCTOR: Dr. Alan J. Jircitano
OFFICE: 33 Hammermill
PHONE: 898-6400
INTERNET: jircitano@psu.edu
http://chemistry.bd.psu.edu/jircitano/
OFFICE HOURS: M 10 - 11, R 4 - 5, F 11 - 12 and by appointment
TEXT: Powerpoint Notes
Crystal Structure Determination - William Clegg

COURSE CONTENT:

1. Overview
2. Crystals
3. Growth
4. Selection
5. Properties
6. Sample Preparation
7. Diffraction of X-rays
8. X-ray Sources
9. Lattices, Planes, and Indices
10. Bragg's Law
11. Reciprocal Space
12. Symmetry Operations and Space Groups
13. Data Collection
14. Geometric
15. Intensity
16. Diffractometers and Computers
17. Data Reduction
18. Structure Factors and Fourier Synthesis
19. The Phase Problem
20. Heavy Atom Method: Patterson Maps and Harker Lines and Planes
21. Direct Methods
22. Refinement
23. Derived Results
24. Computer Programs
25. Structured Solution Software: SHELXS and SHELXL
26. Graphics: ORTEP
27. A Real Crystal Structure
28. 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>Percentage Range</th>
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<tbody>
<tr>
<td>A</td>
<td>100 - 93%</td>
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<tr>
<td>A–</td>
<td>90 - 92%</td>
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<tr>
<td>B+</td>
<td>87 - 89%</td>
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<tr>
<td>B</td>
<td>83 - 86%</td>
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<td>B–</td>
<td>80 - 82%</td>
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<td>C+</td>
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<td>C</td>
<td>70 - 76%</td>
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<td>D</td>
<td>60 - 69%</td>
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<td>F</td>
<td>0 - 59%</td>
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</table>

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.

3. Instructors are asked (Senate rule 49-20) to provide a statement at the beginning of a course to "clarify the application of academic integrity to that course." The Senate Rule includes the following:

   Academic dishonesty includes, but is not limited to, cheating, plagiarizing, fabrication of information or citation, facilitating acts of academic dishonesty by others, having unauthorized possession of examinations, submitting work of another person or work previously used without informing the instructor, or tampering with the work of other students.

Read Senate rule 49-20: [www.psu.edu/ufs/policies/47-00.html#49-20](http://www.psu.edu/ufs/policies/47-00.html#49-20) and Behrend academic integrity guidelines: [www.pserie.psu.edu/faculty/academics/integrity.htm](http://www.pserie.psu.edu/faculty/academics/integrity.htm)

Any violation of academic integrity will receive academic and possibly disciplinary sanctions, including the possible awarding of an XF grade which 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 repeat offenders can be sanctioned accordingly.