CGS Agenda Item: 22-06
Effective Fall 2022

Eastern Illinois University

New/Revised Course Proposal Format

(Approved by CAA on 4/3/14 and CGS on 4/15/14, Effective Fall 2014)

Banner/Catalog Information (Coversheet)

1. __X__ **New Course or** _____ **Revision of Existing Course**
2. **Course prefix and number:** CHM 4780
3. **Short title:** X-ray Crystallography
4. **Long title:** X-ray Crystallography
5. **Hours per week:** 2 Class 3 Lab 3 Credit
6. **Terms:** X Fall ___ Spring ___ Summer ___ On demand
7. **Initial term**: X Fall ___ Spring ___ Summer Year: 2022
8. **Catalog course description:**

   This course is designed to give students an understanding of X-ray crystallography, including the history, theories, and methodology of X-ray diffraction (both powder and single crystal). The lab component of the course will provide students with hands on experience synthesizing crystals, mounting crystals, initializing data collections, solving crystal structures, along with the collection, solving, and analyzing of powder and single-crystal X-ray diffraction patterns. The course also provides students with a background in preparing crystallographic information files (.cif) which are submitted with any crystal structure publication, preparing data and figures for publication, and the writing that goes along with preparing a crystal structure for publication.

9. **Course attributes:**

   General education component: N/A

   ___ Cultural diversity ___ Honors __ Writing centered _____ Writing intensive __X__ Writing active

10. **Instructional delivery**
    Type of Course:

    ___ Lecture ___ Lab X Lecture/lab combined ___ Independent study/research

    ___ Internship ___ Performance ___ Practicum/clinical ___ Other, specify: _____

    Mode(s) of Delivery:

    __X__ Face to Face ___ Online ___ Study Abroad

    ___ Hybrid, specify approximate amount of on-line and face-to-face instruction _____

11. Course(s) to be deleted from the catalog once this course is approved.
    None

12. **Equivalent course(s):** None

    a. Are students allowed to take equivalent course(s) for credit? _____ Yes _____ No

13. **Prerequisite(s):** CHM 1410 and CHM 1415

    a. **Can prerequisite be taken concurrently?** ___ Yes X No

    b. **Minimum grade required for the prerequisite course(s)?** C

    c. **Use Banner coding to enforce prerequisite course(s)?** X Yes ___ No

    d. **Who may waive prerequisite(s)?**

    ___ No one X Chair ___ Instructor ___ Advisor ___ Other (specify)

14. **Co-requisite(s):** N/A

15. **Enrollment restrictions**

    a. **Degrees, colleges, majors, levels, classes which may take the course:** All

    b. **Degrees, colleges, majors, levels, classes which may not take the course:** None

16. **Repeat status:** X May not be repeated ___ May be repeated once with credit

17. **Enter the limit, if any, on hours which may be applied to a major or minor:** 3

18. **Grading methods:** X Standard ___ CR/NC Audit ___ ABC/NC

19. **Special grading provisions:**

    ___ Grade for course will not count in a student's grade point average.

    ___ Grade for course will not count in hours toward graduation.

    ___ Grade for course will be removed from GPA if student already has credit for or is registered in: _____

    ___ Credit hours for course will be removed from student's hours toward graduation if student already has credit for or is registered in: _____

20. **Additional costs to students:**
    Supplemental Materials or Software $0

    Course Fee ___ No X Yes, Explain if yes $35, for chemicals used in the laboratory experiments and consumable materials for the X-ray diffractometer (which will be used in the class)

21. **Community college transfer:**

    ___ A community college course may be judged equivalent.

    X A community college may not be judged equivalent.

    Note: Upper division credit (3000+) will not be granted for a community college course, even if the content is judged to be equivalent.

Rationale, Justifications, and Assurances (Part I)

1. __Course is required for the major(s) of _____
   ___Course is required for the minor(s) of _____
   ___Course is required for the certificate program(s) of _____
   __X__Course is used as an elective
2. **Rationale for proposal** :
   This course has been offered previously as a very popular special topics course (CHM 4800), and the chemistry department has currently used up the number of times it can be offered as a special topics class. This is a unique course, unable to be offered at many PUIs due to lack of expensive instrumentation, which gives students the chance to work hands on with crystal growth, data collection, and data analysis using a single crystal X-ray diffractometer. Single crystal X-ray diffraction is a technique that is widely used in chemical industry, such as in pharmaceutical companies to classify and study drug compounds, determine absolute stereochemistry of a drug, which is extremely important, and to determine purity of synthesized samples. This technique is used in research to solve the exact structure of the product produced in all manners of chemistry groups from physical chemistry, organic chemistry, biochemistry, and inorganic chemistry. Additionally, this course will increase the number of undergraduate fall chemistry electives from one to two, and it will also be offered as a graduate course to MS students in both the thesis and non-thesis degree options. As the topics in this course expand past chemistry, this course will also be advertised in the geology department. This course has been very popular in the past, and the department has received several inquires from students about when this course will be offered again, so it is expected that this course will attract undergraduate students from chemistry and geology, as well as graduate students from chemistry. This course would initially be offered every-other-year, in rotation with other chemistry electives.
3. **Justifications for (answer N/A if not applicable)**
   Similarity to other courses: N/APrerequisites: As some basic knowledge of chemistry and chemical structures is needed, completion of the general chemistry sequence is required.
   Co-requisites: N/A
   Enrollment restrictions: N/A
   Writing active, intensive, centered: As the students are required to write a crystal structure report as well as written portions on the laboratory assignments, a writing active designation is deemed appropriate.
4. **General education assurances (answer N/A if not applicable)**
   General education component: N/A

Curriculum: N/A

Instruction: N/A

Assessment: N/A

5. **Online/Hybrid delivery justification & assurances (answer N/A if not applicable)**

Online or hybrid delivery justification: N/A

Instruction: N/A

Integrity: N/A

Interaction: N/A

Model Syllabus (Part II)

Please include the following information:

1. Course number and title

CHM 4780, X-ray Crystallography

2. Catalog description

This course is designed to give students an understanding of X-ray crystallography, including the history, theories, and methodology of X-ray diffraction (both powder and single crystal). The lab component of the course will provide students with hands on experience synthesizing crystals, mounting crystals, initializing data collections, solving crystal structures, along with the collection, solving, and analyzing of powder and single-crystal X-ray diffraction patterns. The course also provides students with a background in preparing crystallographic information files (.cif) which are submitted with any crystal structure publication, preparing data and figures for publication, and the writing that goes along with preparing a crystal structure for publication.

3. Learning objectives.

Undergraduate students enrolled will develop and demonstrate knowledge and competencies in thefollowing areas:

- Historical importance and fundamental laws of X-ray diffraction (CT2-3, CT5, WR3-4, WR-7, SL1, QR1, QR3)
- Crystal systems and centering conditions from unit cell parameters or space groups (CT2-4, WR4, WR7, QR1, QR3)
- Theory and methodology of single-crystal X-ray crystallography (SCXRD) and powder X-ray diffraction (PXRD) (CT2-5, WR4-5, WR7, QR1-3)
- Interpretation of crystallographic data (CT2-6, WR2-5, WR7, SL3-4, QR1-6)
- Assessment and critique of crystallographic data (CT2, CT4, WR4, WR7, QR1-6)
- Common X-ray diffraction instrumentation and software (CT2, CT4, WR4, WR7, QR1-6)
- Hands on structure solution and refinement using EIU's X-ray diffractometer (CT2-4, CT6, WR4, WR7, SL2-3, QR1-6)
- Preparing X-ray data for publication in a peer-reviewed journal (CT2-4, CT6, WR1-7, SL1-3, QR-1-6)
- Presenting and evaluating X-ray data (CT2-6, WR1-7, SL1-7, QR-1-6)

Graduate students enrolled will develop and demonstrate knowledge and competencies in the following areas:

- Historical importance and fundamental laws of X-ray diffraction (1. Depth of content knowledge; 2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills)
- Crystal systems and centering conditions from unit cell parameters or space groups (1. Depth of content knowledge; 2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills)
- Theory and methodology of single-crystal X-ray crystallography (SCXRD) and powderX-ray diffraction (PXRD) (1. Depth of content knowledge; 2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills)
- Interpretation of crystallographic data (1. Depth of content knowledge; 2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills)
- Assessment and critique of crystallographic data (1. Depth of content knowledge; 2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills; 4. Evidence of advanced scholarship through research and/or scholarship activity)
- Common X-ray diffraction instrumentation and software (1. Depth of content knowledge; 2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills)
- Hands on structure solution and refinement using EIU's X-ray diffractometer (1. Depth of content knowledge; 2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills; 4. Evidence of advanced scholarship through research and/or scholarship activity)
- Preparing X-ray data for publication in a peer-reviewed journal (2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills; 4. Evidence of advanced scholarship through research and/or scholarship activity; 5. Ethical and professional responsibility)
- Presenting and evaluating X-ray data (2. Critical thinking and problem solving skills; 3. Effective oral and written communication skills; 4. Evidence of advanced scholarship through research and/or scholarship activity; 5. Ethical and professional responsibility)

4. Course materials.

Crystal Structure Determination. W. Massa, 2004, Springer.
Principles of X-Ray Crystallography. L. Ooi, 2010, Oxford University Press.
Other materials will be made available on a Learning Management System (LMS).

5. Weekly outline of content.

Week	Topic	Textbook Readings (pg)	
		Massa	**Ooi**
Week 1	Course Introduction		
	History of X-Ray Crystallography		
	An introduction to the method of X-Ray Crystallography: Crystal Growth	1, 67-69	3-10, 112-114
Week 2	Lattice Points and Unit Cells	3-6	11-16
	Unit Cells and Fractional Coordinates	See handout(s)	
Week 3	Point and Space Symmetries: Rotational Symmetry and the 7 Crystal Systems	6-11, 41-51	36-39, 44-47
	Symmetry: Mirror Planes, Inversion, Rotary Inversion	41-65	39-40
	Symmetry: Screw Aces and Glide Planes	41-65	40-44
Week 4	Symmetry: Centering and Bravais Lattices	41-65	17-21
	Space Groups: Combining Symmetry Operations	41-65	44-47, 48-86
	Introduction to Crystallographic Programs	See handout(s)	
Week 5	Exam 1		
	Space Groups: Interpretation of Symbols	56-61	54-65

Week 6	Space Groups: Using Space Group Information and the International Tables	52-56	61-65
	Crystallographic Directions, Planes, Faces, and Forms	20-22	26-28
Week 7	Introduction to Solving Structures in Apex3	See handout(s)	
Week 8	X-Ray Generation and Detection	71-92	115-119
Week 9	Powder X-Ray Diffraction	124-125	
	Exam 2		
Week 10	Diffraction of X-rays	22-23, 27-31	30-35, 126-127
Week 11	Diffraction Intensity Data	33, 37, 89-91	119-123
	Solving the structure: Symmetry determination	62-65	67-80
Week 12	Solving the structure: Locating the first atoms	93-109	81-92
	Solving the structure: Structure refinement	111-125	93-100
Week 13	Exam 3		
	Solving the Structure: Derived Results	161-170	105-111
Week 14	Solving the Structure: Challenging Problems – Disorder and Twinning	126-132, 145-159	100-102
	X-Ray Databases	171-176	
	Special Topics: Protein Crystallography		
Week 15	Student Presentations		
Finals Week	**Final Exam**		

Lab Outline:

Experiment	**Experiment Due**
Macroscopic Evaluation of Crystals (Experiment # 1)	
Crystal Growth Methods: Hydrothermal, Fast, and Slow Crystal Growth (Experiment # 2 – Week 1)	Exp. # 1
Crystal Growth Methods: Hydrothermal, Fast, and Slow Crystal Growth (Experiment # 2 – Week 2)	
Crystal Growth Methods: Hydrothermal, Fast, and Slow Crystal Growth (Experiment # 2 – Week 3)	
Analyzing Crystal Structures (Experiment # 3 – Week 1)	Exp. # 2
Analyzing Crystal Structures (Experiment # 3 – Week 2)	
Chiral Crystallization of Ethylene Diamine Sulfate (Experiment # 4)	Exp. # 3
Solving the Structures of Simple Molecules (Experiment # 5)	Exp. # 4
Identification of an Unknown Household Solid by X-Ray Powder Diffraction (Experiment # 6)	Exp. # 5
Solving the Structures of More Complex Organic Molecules (Experiment # 7)	Exp. # 6
Solving Crystal Structures for Student Presentations	Exp. # 7
Solving Disorder in Crystal Structures (Experiment # 8)	
Case Study Lab (Experiment # 9 – Week 1)	Exp. # 8
Case Study Lab Discussion (Experiment # 9 – Week 2)	Exp. # 9
Lab Checkout and Make-up Labs as needed	

6. Assignments and evaluation, including weights for final course grade.

50-minute Examinations (3)	30%
Homework Assignments (5-12)	15%
Student Presentation (1) 15-minutes (Graduate Students) 10-minutes (Undergraduate Students)	10%
Crystal Structure Report (1) (Acta E Style Undergraduate Students) (Chemical Communication style Graduate Students)	10%
Laboratory Assignments (9)	20%
Final Examination (1)	15%

7. Grading scale.

≥ 87%	A
86% ≥ 75%	B
74% ≥63%	C
62% ≥ 50%	D
< 50%	F

8. Correlation of learning objectives to assignments and evaluation.

Learning Objective	**University Learning Goals Undergraduate** ***Graduate***	**Homework Assignments**	**Student Presentation**	**Student Report**	**Laboratory Assignments**	**Exams**	**Final Exam**
Grade Percentage		(15%)	(10%)	(10%)	(20%)	(30%)	(15%)
Historical importance and fundamental laws of X-ray diffraction	CT2-3, CT5, WR3-4, WR-7, SL1, QR1, QR3 *1, 2, 3*	X			X	X	X
Crystal systems and centering conditions from unit cell parameters or space groups	CT2-4, WR4, WR7, QR1, QR3 *1, 2, 3*	X	X	X	X	X	X
Theory and methodology of single-crystal X-ray crystallography (SCXRD) and powder X-ray diffraction (PXRD)	CT2-5, WR4-5, WR7, QR1-3 *1, 2, 3*	X	X	X	X	X	X
Interpretation of crystallographic data	CT2-6, WR2-5, WR7, SL3-4, QR1-6 *1, 2, 3*	X	X	X	X	X	X
Assessment and critique of crystallographic data	CT1-6, WR1-7, SL-1, SL2-3, QR1-6 *1, 2, 3, 4*	X	X	X	X	X	X

Common X-ray diffraction instrumentation and software	CT2, CT4, WR4, WR7, QR1-6 *1, 2, 3*	X	X	X	X	X	X
Hands on structure solution and refinement using EIU's X-ray diffractometer	CT2-4, CT6, WR4, WR7, SL2-3, QR1-6 *1, 2, 3, 4*		X	X	X		
Preparing X-ray data for publication in a peer-reviewed journal	CT2-4, CT6, WR1-7, SL1-3, QR-1-6 *2, 3, 4, 5*		X	X	X		
Presenting and evaluating X-ray data	CT2-6, WR1-7, SL1-7, QR-1-6 *2, 3, 4, 5*		X	X	X		

Date approved by the department or school: 12/3/2021
Date approved by the college curriculum committee: 2/2/22
Date approved by the Honors Council *(if this is an honors course):*
Date approved by CAA: CGS: