NEW COURSE FORM

(*denotes required fields)

1. General Information

a. * Submitted by the College of:

COLLEGE OF ARTS & SCIENCES Today's Date: 3/5/2012

b. * Department/Division:

Chemistry

c.

***** Contact Person Name:	Mark Meier	Email:	meier@uky.edu
		Phone:	257-7082
***** Responsible Faculty ID (if different from Contact)	Sean Parkin	Email:	s.parkin@uky.edu
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d. * Requested Effective Date: ◉ Semester following approval OR ○ Specific Term/Year [1]

e.

Does the change make the course a UK Core course? ○ Yes ◉ No

If YES, check the areas that apply:

☐ Inquiry - Arts & Creativity ☐ Composition & Communications - II

☐ Inquiry - Humanities ☐ Quantitative Foundations

☐ Inquiry - Nat/Math/Phys Sci ☐ Statistical Inferential Reasoning

☐ Inquiry - Social Sciences	☐ U.S. Citizenship, Community, Diversity
☐ Composition & Communications - I	☐ Global Dynamics

2. Designation and Description of Proposed Course.

a. * Will this course also be offered through Distance Learning? ○ Yes [4] ◉ No

b. * Prefix and Number:
CHE 640

c. * Full Title:
Chemical Crystallography

d. Transcript Title (if full title is more than 40 characters):

e. To be Cross-Listed [2] with (Prefix and Number):

f. * Courses must be described by at least one of the meeting patterns below. Include number of actual contact hours[3] for each meeting pattern type.

2 Lecture	2 Laboratory[1]	Recitation	Discussion
Indep. Study	Clinical	Colloquium	Practicum
Research	Residency	Seminar	Studio
Other	If Other, Please explain:		

g. * Identify a grading system: ◉ Letter (A, B, C, etc.) ○ Pass/Fail

h. * Number of credits: 3

i. * Is this course repeatable for additional credit? ○ Yes ◉ No
If YES: Maximum number of credit hours:

If YES: Will this course allow multiple registrations during the same semester? ○ Yes ○ No

j. * Course Description for Bulletin:

An introduction to modern small-molecule crystallography with emphasis on typical applications of interest to synthetic chemists.

k. Prerequisites, if any:

CHE 232 and a physical chemistry course at the 400-level or above,

l. Supplementary teaching component, if any: ○ Community-Based Experience ○ Service Learning ○ Both

3. * Will this course be taught off campus? ○ Yes ◉ No

If YES, enter the off campus address:

4. Frequency of Course Offering.

a. * Course will be offered (check all that apply): ☐ Fall ☑ Spring ☐ Summer ☐ Winter

b. * Will the course be offered every year? ○ Yes ◉ No

If No, explain:

Offering this course as a CHE 580 in alternate years worked well.

5. * Are facilities and personnel necessary for the proposed new course available? ◉ Yes ○ No

If No, explain:

6. * What enrollment (per section per semester) may reasonably be expected? 8

7. Anticipated Student Demand.

a. * Will this course serve students primarily within the degree program? ◉ Yes ○ No

b. * Will it be of interest to a significant number of students outside the degree pgm? (•) Yes ( ) No

If YES, explain:

This course should be of interest to PHYS and Pharmacy students.

8. **Check the category most applicable to this course:**

[x] Traditional – Offered in Corresponding Departments at Universities Elsewhere
[ ] Relatively New – Now Being Widely Established
[ ] Not Yet Found in Many (or Any) Other Universities

9. **Course Relationship to Program(s).**

a. * Is this course part of a proposed new program? ( ) Yes (•) No

If YES, name the proposed new program:

b. * Will this course be a new requirement [5] for ANY program? ( ) Yes (•) No

If YES [5], list affected programs::

10. **Information to be Placed on Syllabus.**

a. * Is the course 400G or 500? ( ) Yes (•) No

If YES, the *differentiation for undergraduate and graduate students must be included* in the information required in **10.b**. You must include: (i) identification of additional assignments by the graduate students; and/or (ii) establishment of different grading criteria in the course for graduate students. (See SR 3.1.4.)

b. [ ] * The syllabus, including course description, student learning outcomes, and grading policies (and 400G-/500-level grading differentiation if applicable, from **10.a** above) are attached.

[1] Courses are typically made effective for the semester following approval. No course will be made effective until all approvals are received.

[2] The chair of the cross-listing department must sign off on the Signature Routing Log.

[3] In general, undergraduate courses are developed on the principle that one semester hour of credit represents one hour of classroom meeting per week for a semester, exclusive of any laboratory meeting. Laboratory meeting, generally, represents at least two hours per week for a semester for one credit hour. (from SR 5.2.1)

[4] You must also submit the Distance Learning Form in order for the proposed course to be considered for DL delivery.

[5] In order to change a program, a program change form must also be submitted.

Rev 8/09

Graduate Council 5/3/12 Brian Jackson

Chemical Crystallography

CHE 640 (section number TBA)

Instructor – Dr. Sean Parkin

CP135 Chemistry Physics Building
Department of Chemistry
Lexington, KY, 40506-0055

office: 323-8984
e-mail: s.parkin@uky.edu
office hours: TBA

Course Overview

This course will be an introduction to structure determination by X-ray diffraction. It is intended to be suitable for graduate and advanced undergraduate students whose primary area of interest is either synthetic organic, inorganic or organometallic chemistry. It could also be of benefit to students of physics and pharmacy.

The course does not revolve around any particular textbook, but the following books cover most of the material reasonably well. The first book is purely an introduction and should be sufficient, while the second is very much more involved.

"Crystal Structure Determination" by Werner Massa
English translation by Gould
Springer: ISBN 3-540-65970-6

"Fundamentals of Crystallography" by Carmelo Giacovazzo
Oxford University Press: ISBN 0-19-855578-4

The general progression of the course will loosely follow the steps involved in a typical routine structure determination, but will also introduce concepts necessary for a deeper understanding of the subject. The nature of the material requires that some mathematical derivations be presented, but these will be kept to a minimum. The general level of mathematics required for a typical bachelors degree in chemistry should be sufficient.

There will be homework assignments (most weeks) as well as midterm exams and a final project.

The real intent of the course is to provide sufficient background information that students can collect X-ray diffraction data, solve and refine a relatively well-behaved small-molecule crystal structure. To this end there will be regular sessions in the X-ray laboratory either in groups or individually to allow hands-on exposure to the diffraction equipment and computers.

Lecture and lab attendance is absolutely mandatory. Absences require the consent of the instructor. This rule applies to people taking the course for credit and audit.

Course Requirements

Assignment of grades for this course will be based upon homework problem sets, a midterm exam and the successful completion and write up (as if for publication in the electronic journal Acta-Crystallographica, Section E) of a crystal structure determination. The latter will constitute the final exam and can be started after the mid-term exam, *i.e.*, as soon as a student feels ready to tackle semi-independent practical work. Crystals for this “final exam” may be from the student’s own research project.

Homework assignments and the mid-term exam will contribute 25% each of the total score for the course, with the remaining 50% from the “final.” Grades will be assigned according to the following scheme.

A:	85	<score≤	100%
B:	70	<score≤	85%
C:	55	<score≤	70%
E	0	<score≤	55%

Since graduate students cannot receive a "D" grade, an "E" grade is anything below 55%.

Collaboration on homework assignments is allowed but verbatim copying is not. Collaboration on the midterm is not allowed, but reference to books, lecture notes, journals, *etc*. is fine (it will be a take home exam). The ultimate goal of the course is to get the student comfortable with crystallography, competent to determine simple structures and capable of describing and interpreting published work. To this end, collaboration with others is encouraged and help from the instructor is available (as a last resort and within reason) during the final project. Students will be required to adhere strictly to the CIF (crystallographic information file) format when they write up the final structure report.

Excused Absences (boilerplate):

Students need to notify the professor of absences prior to class when possible. S.R. 5.2.4.2 defines the following as acceptable reasons for excused absences: (a) serious illness, (b) illness or death of family member, (c) University-related trips, (d) major religious holidays, and (e) other circumstances found to fit “reasonable cause for nonattendance” by the professor.

Students anticipating an absence for a major religious holiday are responsible for notifying the instructor in writing of anticipated absences due to their observance of such holidays no later than the last day in the semester to add a class. Information regarding dates of major religious holidays may be obtained through the religious liaison, Mr. Jake Karnes (859-257-2754).

Students are expected to withdraw from the class if more than 20% of the classes scheduled for the semester are missed (excused or unexcused) per university policy.

Verification of Absences (boilerplate):

Students may be asked to verify their absences in order for them to be considered excused. Senate Rule 5.2.4.2 states that faculty have the right to request "appropriate verification" when students claim an excused absence because of illness or death in the family. Appropriate notification of absences due to university-related trips is required prior to the absence.

Academic Integrity (boilerplate):

Per university policy, students shall not plagiarize, cheat, or falsify or misuse academic records. Students are expected to adhere to University policy on cheating and plagiarism in all courses. The minimum penalty for a first offense is a zero on the assignment on which the offense occurred. If the offense is considered severe or the student has other academic offenses on their record, more serious penalties, up to suspension from the university may be imposed.

Plagiarism and cheating are serious breaches of academic conduct. Each student is advised to become familiar with the various forms of academic dishonesty as explained in the Code of Student Rights and Responsibilities. Complete information can be found at the following website: http://www.uky.edu/Ombud. A plea of ignorance is not acceptable as a defense against the charge of academic dishonesty. It is important that you review this information as all ideas borrowed from others need to be properly credited.

Part II of *Student Rights and Responsibilities* (available online http://www.uky.edu/StudentAffairs/Code/part2.html) states that all academic work, written or otherwise, submitted by students to their instructors or other academic supervisors, is expected to be the result of their own thought, research, or self-expression. In cases where students feel unsure about the question of plagiarism involving their own work, they are obliged to consult their instructors on the matter before submission.

When students submit work purporting to be their own, but which in any way borrows ideas, organization, wording or anything else from another source without appropriate acknowledgement of the fact, the students are guilty of plagiarism. Plagiarism includes reproducing someone else's work, whether it be a published article, chapter of a book, a paper from a friend or some file, or something similar to this. Plagiarism also includes the practice of employing or allowing another person to alter or revise the work which a student submits as his/her own, whoever that other person may be.

Students may discuss assignments among themselves or with an instructor or tutor, but when the actual work is done, it must be done by the student, and the student alone. When a student's assignment involves research in outside sources of information, the student must carefully acknowledge exactly what, where and how he/she employed them. If the words of someone else are used, the student must put quotation marks around the passage in question and add an appropriate indication of its origin. Making simple changes while leaving the organization, content and phraseology intact is plagiaristic. However, nothing in these Rules shall apply to those ideas which are so generally and freely circulated as to be a part of the public domain (Section 6.3.1).

Please note: Any assignment you turn in may be submitted to an electronic database to check for plagiarism.

Accommodations due to disability (boilerplate):

If you have a documented disability that requires academic accommodations, please see me as soon as possible during scheduled office hours. In order to receive accommodations in this course, you must provide me with a Letter of Accommodation from the Disability Resource Center (Room 2, Alumni Gym, 257-2754, email address: jkarnes@email.uky.edu) for coordination of campus disability services available to students with disabilities.

CHE640 - Chemical Crystallography

MAJOR TEACHING OBJECTIVES

1) To provide students with a working knowledge of small-molecule crystallographic equipment.

2) To provide students with a working knowledge of small-molecule crystallographic software for structure solution, refinement and presentation.

3) To provide students with sufficient theoretical background to understand what each of the practical aspects (in 1 & 2 above) entail.

4) To provide students with sufficient information that they can understand crystallographic information presented in the literature.

LEARNING OUTCOMES

On completion of this course, a highly successful student will be able to do the following:

1) Grow crystals from the products of their (or others) synthetic chemistry research.

2) Inspect the crystals and quickly decide whether any of the crystals are usable for structure determination.

3) Mount a suitable crystal, collect high quality x-ray diffraction data, and process that data for structure determination.

4) Solve and refine routine crystal structures.

5) Prepare routine crystal structures for publication.

6) Interpret and describe crystallographic results with authority, *e.g.* at a scientific meeting.

7) Use the common crystallographic databases to search and extract results relevant to their own research.

Chemical Crystallography – CHE 640

Syllabus

1) Concepts - What are crystals and x-rays ?

2) Brief History

3) Crystal Growth

a) Evaporation

b) Slow cooling

c) Vapour diffusion

d) Solvent diffusion

e) Convection

f) Sublimation

g) Melt

h) Others

4) Crystal Selection

    a) Size

    b) Shape

    c) General appearance

5) Crystal Lattices and Lattice Symmetry

    a) Seven crystal systems

    b) Fourteen Bravais lattices

    c) Unit cell

d) Asymmetric unit

e) Direct and Reciprocal Lattices

6) X-Ray Generation

    a) Sealed tube

    b) Rotating anode
    c) Synchrotron
    d) X-Ray optics

7) X-ray Detectors
    a) Scintillation counters (serial diffractometers)
    b) Area detectors

8) Diffraction Geometry
    a) Bragg's law
    b) Laue equations
    c) Ewald sphere
    d) Four circle geometry - "symmetric" mode serial diffractometer
    e) Rotation geometry - modern "area detectors"
    f) Friedel's law

9) Fourier Theory

10) Structure Factors and Electron Density

11) Space Group Symmetry
    a) Hermann-Mauguin versus Schönflies notation
    b) Inversion points
    c) Pure rotation
    d) Improper rotation (roto-inversion)
    e) Mirror planes
    f) Screw axes
    g) Glide planes
    h) How to read the International Tables

12) Data Collection
    a) Indexing

- b) Counting statistics
- c) Low temperature versus room temperature
- d) Unique data
- e) Redundancy

13) Data Reduction

- a) Lorentz and polarization corrections
- b) Integration of intensities
- c) Scaling and merging of intensities

14) Space group determination

- a) Lattice centering
- b) Systematic absences
- c) Effect of lattice symmetry on the weighted reciprocal lattice

15) Structure Solution and the Phase Problem

- a) Direct methods
- b) Patterson methods

16) Structure Refinement

- a) Least-squares refinement
- b) Difference Fourier synthesis
- c) Displacement "thermal" parameters
- d) Hydrogen atoms

17) Problems

- a) Absorption
- b) Extinction
- c) Thermal diffuse scattering

d) Renninger effects

e) $\lambda/2$ effects

f) Libration

g) Spherical scattering factor approximation

h) Disorder

i) Twinning

j) Anomalous Dispersion and Absolute Configuration

18) Crystallographic Literature and Databases

a) Thermal ellipsoid plots

b) Interpreting crystal structure reports

c) Cambridge Structure Database

d) Protein Data Bank