APPLICATION FOR NEW COURSE

1. Submitted by the College of Arts and Sciences ____________________________ Date: 2-12-09

Department/Division proposing course: Chemistry

2. Proposed designation and Bulletin description of this course:
   a. Prefix and Number CHEM 540
   b. Title Chemical Crystallography
      *If title is longer than 24 characters, offer a sensible title of 24 characters or less:

   c. Courses must be described by at least one of the categories below. Include number of actual contact hours per week.
      ( ) CLINICAL ( ) COLLOQUIUM ( ) DISCUSSION ( ) LABORATORY ( ) LECTURE
      ( ) INDEPENDENT STUDY ( ) PRACTICUM ( ) RECITATION ( ) RESEARCH ( ) RESIDENCY
      ( ) SEMINAR ( ) STUDIO ( ) OTHER – Please explain: ____________________________

   d. Please choose a grading system: (x) Letter (A, B, C, etc.) ( ) Pass/Fail

   e. Number of credit hours: 3.0

   f. Is this course repeatable? (x) YES ( ) NO
      If YES, maximum number of credit hours: __________________

   g. Course description:
      An introduction to modern small molecule crystallography with emphasis on typical applications of interest to synthetic chemists.

   h. Prerequisite(s), if any:
      CHEM 232 and a physical chemistry course at the 400 level or above, or consent of instructor.

   i. Will this course also be offered through Distance Learning? (x) YES ( ) NO
      If YES, please check one of the methods below that reflects how the majority of the course content will be delivered:
      Internet/Web-based ( ) Interactive video ( ) Extended campus ( )

3. Supplementary teaching component: (x) N/A or ( ) Community-Based Experience ( ) Service Learning ( ) Both

4. To be cross-listed as:

   Prefix and Number ____________________________

   printed name ____________________________

   Cross-listing Department Chair ____________________________

   signature ____________________________

5. Requested effective date (term/year): Spring ___________ / 2010

6. Course to be offered (please check all that apply): ( ) Fall (x) Spring ( ) Summer
APPLICATION FOR NEW COURSE

7. Will the course be offered every year? ☒ YES ☐ NO
   If NO, please explain: ____________________________________________________________

8. Why is this course needed?
   Graduate chemists need experience with x-ray crystallography so that they can determine molecular structures and interpret other work.

9. a. By whom will the course be taught? Dr. Sean Parkin
    ☒ YES ☐ NO
   b. Are facilities for teaching the course now available?
      If NO, what plans have been made for providing them?
      ____________________________________________________________

10. What yearly enrollment may be reasonably anticipated?
    Due to the lab component, this must be capped at 10, with typical enrollment at 8.

11. a. Will this course serve students primarily within the department? ☒ Yes ☐ No
    b. Will it be of interest to a significant number of students outside the department? ☒ YES ☐ NO
       The precursor to the proposed course usually has a few students from Physics, Pharmacy, or both.

12. Will the course serve as a University Studies Program course? ☐ YES ☒ NO
   If YES, under what Area?
   ☐ YES ☒ NO
   "AS OF SPRING 2007, THERE IS A MORATORIUM ON APPROVAL OF NEW COURSES FOR USP."

13. Check the category most applicable to this course:
    ☒ traditional – offered in corresponding departments at universities elsewhere
    ☐ relatively new – now being widely established
    ☐ not yet to be found in many (or any) other universities

14. Is this course applicable to the requirements for at least one degree or certificate at UK? ☒ Yes ☐ No

15. Is this course part of a proposed new program?
    If YES, please name: ____________________________________________________________
    ☐ YES ☒ NO

16. Will adding this course change the degree requirements for ANY program on campus?
    If YES, list below the programs that will require this course:
    ☐ YES ☒ NO

   "In order to change the program(s), a program change form(s) must also be submitted."
17. ☑ The major teaching objectives of the proposed course, syllabus and/or reference list to be used are attached.

18. ☑ Course is 400G or 500G. If the course is 400G- or 500-level, you must include a syllabus showing differentiation for undergraduate and graduate students by (i) requiring additional assignments by the graduate students; and/or (ii) the establishment of different grading criteria in the course for graduate students. (See SR 3.1.4)

19. Within the department, who should be contacted for further information about the proposed new course?

Name: Dr. Sean Parkin  Phone: 3-8984  Email: s.parkin@uky.edu

20. Signatures to report approvals:

May 11, 2009  Printed name  Reported by Department Chair

DATE of Approval by Department Faculty

9/22/09  Printed name  Reported by College Dean

DATE of Approval by College Faculty

11/3/2009  Printed name  Reported by Undergraduate Council Chair

*DATE of Approval by Undergraduate Council

*DATE of Approval by Graduate Council

*DATE of Approval by Health Care Colleges Council (HCCC)

*DATE of Approval by Senate Council

*DATE of Approval by University Senate

*If applicable, as provided by the University Senate Rules. (http://www.uky.edu/USC/New/RulesandRegulationsMain.htm)
INVESTIGATING AREA: Natural & Math. Sci.  COURSE MAJOR, DEGREE or PROGRAM: 

DATE FOR EPC REVIEW: Sep 22 2009  CATEGORY: NEW, CHANGE, DROP  Che 540

INSTRUCTIONS: This completed form will accompany the course application to the Graduate/Undergraduate Council(s) in order to avoid needless repetition of investigation. The following questions are included as an outline only. Be as specific and as brief as possible. If the investigation was routine, please indicate this. The term “course” is used to indicate one course, a series of courses or a program, whichever is in order. Return the form to the Office of the Associate Dean, 275 Patterson Office Tower for forwarding to the Council(s). ATTACH SUPPLEMENT IF NEEDED.

1. List any modifications made in the course proposal as submitted originally and why.

   1. Clarification of grading scheme for graduate students.
   2. Clarification of response to C14 - course is an option in program not required.

2. If no modifications were made, review considerations that arose during the investigation and the resolutions. 

3. List contacts with program units on the proposal and the considerations discussed therein.
   Dr. Sean Parkin - see att 1 above

4. Additional information as needed.

5. A&S Area Coordinator Recommendation:
   
   ![Approve]

6. A&S Education Policy Committee Recommendation:
   
   ![Approve]

7. Date: 22 Sep 2009

Ruth Beattie, rheat@uky.edu 257-7647

Need to add 11 of contact hours.
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.

<table>
<thead>
<tr>
<th>Grade</th>
<th>Score</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>85</td>
<td>100%</td>
</tr>
<tr>
<td>B</td>
<td>70</td>
<td>85%</td>
</tr>
<tr>
<td>C</td>
<td>55</td>
<td>70%</td>
</tr>
<tr>
<td>D</td>
<td>40</td>
<td>55%</td>
</tr>
<tr>
<td>E</td>
<td>0</td>
<td>40%</td>
</tr>
</tbody>
</table>

*Graduate students cannot receive a "D" grade, so for graduate students, an "E" grade is anything below 55%. Undergraduates are required to complete eight assignments, while graduate students must complete ten. Graduate students also have an additional requirement for their final exam. in that they are required to adhere strictly to the CIF (Crystallographic Information File) format for their final reports.*

Collaboration on homework assignments is allowed but verbatim copying is not. Collaboration on the mid-term 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. The requirements for graduate students differ from those of undergraduates in that graduate students will be required to complete two additional homework assignments and to adhere strictly to the CIF (crystallographic information file) format when they write up the final structure report. Undergraduates will not be bound by this (somewhat severe) restriction.

Undergraduates will be provided with a Midterm Evaluation (by the date of the midterm) of course performance.
Plagiarism, cheating and any other violations of academic integrity will result in an "E" grade for the course.

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.

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 540

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) 1/2 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
Grading Scale for Graduate Students

100-90% = A  
89.9-80% = B  
79.9-70% = C  
< 69.9% = E