

## Ph. D. Guidelines for Physical Chemistry Students at UW-Madison

This document summarizes, with an informal chronological overview, the requirements and expectations for physical chemistry students seeking a Ph.D. in chemistry. It provides both general advice and detailed instructions, and will be helpful to first-year students as well as to advanced students. Please send corrections and suggestions to the pchem divisional chair.

### During the **First Year...**

#### *Fall Semester*

- Talks describing physical chemistry research in various groups are given by faculty in the first part of the Fall semester. You should register for 5 credits of Chem. 992 and attend these talks.
- After these research talks, you should start thinking about choosing a major professor. You are required to interview at least three prospective major professors. Major professors are allowed to make commitments beginning November 1. Under normal circumstances, you should choose a major professor by November 15. Please submit your research group selection document to Pat Houtsinger in the physical chemistry division office in room 8305g.
- After a research group has been selected, you will become involved with the activities of the group, and, as soon as feasible, begin research.
- You are expected to complete the graduate courses Chem. 661 (Chemical and Statistical Thermodynamics) and Chem. 675 (Introductory Quantum Chemistry) in your first semester.
- In the fall of the first year and in all subsequent years, you are expected to register for Chem. 960 for zero credits and attend the weekly physical chemistry seminars.
- All chemistry graduate students are expected to attend Chem. 901 (Seminar- Teaching of Chemistry). This one-credit course will provide information about our graduate program, teaching, choosing an advisor, and future employment.
- You are encouraged to attend the student-run physical chemistry seminars on Tuesday afternoons. In subsequent years, you may present your research in this seminar series.

#### *Spring Semester*

- All chemistry graduate students are required to take the department's Laboratory Safety Course (Chem. 607) during their first year. This course meets during the week preceding the beginning of the spring semester.
- You are expected to enroll in Chem. 960 (Physical Chemistry Seminar) for two-credits (not zero). You should also continue with the spring semester of Chem. 901.

- You will begin taking additional courses, which are chosen in consultation with the your major professor. A total of **10** credits of graduate coursework in physical chemistry (see attached list) is required for a Ph. D. in physical chemistry. In addition, you must satisfy the minor requirement of the graduate school by taking a minimum of **10** graduate credits (some of which can be in physical chemistry) in courses outside of your specialized field. Physical chemistry courses outside of your specialized field may count for credit for the minor requirement and the physical chemistry course requirement, upon approval by your major professor. Chem. 661 and Chem. 675 may not *both* be counted in this way.

In choosing courses, please note that Chem. 661 (3 credits), Chem. 675 (3 credits), and Chem. 960 (2 credits) add up to 8 credits by themselves, leaving a minimum requirement of 2 additional credits in a physical chemistry course. Neither Chem. 901 nor research credits count toward fulfilling the physical chemistry coursework requirement or the graduate school course requirement.

- Registration for the research course 992 or 995 is appropriate in the second and succeeding semesters under the section number for your advisor. You should register for enough research credits to bring the total credit load to 12 as a non-dissertator for the fall and spring semesters and to 2 credits in the summer.

- Students whose major professor has a primary affiliation within the physical chemistry division should enroll in Chem. 964 (Physical Chemistry Group Meetings, now called “Seminar: Molecular Dynamics”) for 0-1 credits each semester during their graduate career. 0 credits given for nominal participation, 1 credit for substantial participation.

### During the **Second Year** ...

- You will continue taking physical chemistry and other courses, chosen in consultation with your major professor.

- Research continues.

- In the first semester all second-year you will take two **Topic Exams**, normally in September and November. For each exam an article (or possibly a few related articles) from the current literature will be identified, and copies will be distributed to you approximately ten days in advance of the exam date. On the exam date you will take a three-hour written exam based on the material in the paper(s) and on the background information necessary to understand it. Exams are graded on a scale of 1 to 5 and additional written work may be assigned to students with grades of 3 or below, at the option of the examining committee. Details are provided at the end of this document.

- In the second semester of your second-year, you will take a **Thesis Background Oral (TBO)** Exam. This TBO involves a 1-2 page written summary (given to the committee three days before the exam) and an oral presentation (approximately 20 minutes) with subsequent questions from a faculty committee. The purpose of the exam is to assess the your preparation for research, including the goals, techniques, and background for the

problem to be addressed. Actual research results are not required, but may be included if available. The committee assigns a grade on a scale of 1 to 5 for the TBO. Students who receive a grade of 3 or lower may be assigned follow-up work or asked to repeat the exam. More details are provided at the end of this document.

**Note:** *please hand deliver your summary to the committee and state the day, time, and location of the oral presentation on the front page*

- The TBO committee will normally also serve as your **mentor committee** (or “thesis committee”) throughout your graduate career. The committee consists of the your major professor and two other faculty members, chosen with input from you. One member of the committee may be from outside the chemistry department.

The mentor committee will evaluate your progress through formal and informal meetings and help guide you through your career. The section beginning on page 8 on the “Ph. D. Program in Chemistry” provides a summary of topics that the committee may discuss with you over your career. We encourage you to consider your committee as a resource to turn to in case any concerns or issues arise during your graduate work that you would like to discuss with faculty other than your major professor.

### During the **Third Year** ...

- Research continues. In collaboration with your major professor, you should prepare and submit manuscripts for publication as appropriate.
- Some specialized courses are not offered every year, and thus it may be appropriate for you to take courses in the third year or beyond.
- At any time following the completion of the TBO, but by the end of the third year, you will prepare and present an **Original Research Proposal (ORP)**. The ORP should involve original research in an area not closely related with your Ph. D. research. The proposal should establish that the proposed research will be of interest and that it is feasible. When your major professor approves the topic, a written proposal and an abstract are prepared. The final step of a successful ORP involves an open oral presentation of 25 minutes or less. After any questions from the audience, you and faculty committee remain and additional questions follow. The divisional secretary should be consulted concerning rules and procedures for scheduling ORPs. Please also see the Graduate Program Coordinator, Stephenie Nagle, room 2108, for the necessary documents three weeks prior to defending. The evaluation committee may be the same as your mentor committee, or you may choose other faculty members closer to the area of the ORP. More details are provided at the end of this document.

**Note:** *please hand deliver your summary to the committee and state the day, time, and location of the oral presentation on the front page*

- After the ORP is defended and dissertator status is achieved, you should register for 3

credits of research (chem. 992 or 995) in the fall, spring, and summer semesters. Continue to enroll for zero credits in Chem. 960 and in Chem. 964. Any other course enrollment should be discussed with your major professor; this enrollment may incur extra tuition charges.

### During the **Fourth Year ...**

- During the spring semester of your 4<sup>th</sup> year, you will meet with members of your Mentor Committee, who will review your progress in research and provide guidance and advice. This 4<sup>th</sup> Year Mentor Committee Review is informal and no grade will be given. You should prepare a 10 minute overview of your research, with particular emphasis on where you will be going and the problems you are facing. The meeting will involve just you and your mentor committee. Please use the first five minutes to bring your Mentor Committee up to speed on your research and the second five minutes to present issues or stumbling blocks that you are now confronting. You may use the black board, prepare a computer presentation, or bring a recent poster with you. During the remaining 20 minutes or so of the meeting, your Mentor Committee will discuss your research with you and your current plans for completing your Ph D. This is an opportune time to talk about any concerns that you may have.

### During the **Fourth and Subsequent Years ...**

- Research continues. In collaboration with your major professor, you should prepare and submit manuscripts for publication as appropriate.
- You will write a **Ph. D. Thesis**, in accordance with Graduate School requirements, and submit it to the major professor for approval.
- You will defend your thesis in a final oral exam. The five-member evaluation committee should include the mentor committee (the major professor and two other faculty members). At least one member of the evaluation committee must be from outside the physical chemistry division or the chemistry department. The final oral exam is to be scheduled at least three weeks in advance; see the Graduate Program Coordinator, Steph Nagle, in room 2108 about Graduate School requirements and forms.
- During the final year you should seek permanent employment or a postdoctoral position. Your major professor, mentor committee, and other members of the department are dedicated to assisting you in your deliberations and search for employment. The Graduate Program Coordinator officer can provide sample CVs and information about industrial interviews. In addition, the department frequently sponsors events that bring employers and students together in the department.

### **Some Notes on Satisfactory Progress**

All Graduate School and Chemistry Department requirements must be met, including taking the Advisory Exams and accumulating enough credits to satisfy the Residence

Requirement (see below). The Graduate School requires that your grade point average be at least 3.0 (not including research credits) each semester in order to maintain satisfactory progress. They also require an overall GPA of at least 3.0 to receive a Ph. D. degree. Classes with grades of BC or C may be used to satisfy the 10 credit university minor requirement and the 10 credit pchem course requirement if they are offset by a combination of grades of AB and A to maintain a GPA of at least 3.0.

### **Check List for Registration, Classes, and Forms**

As a non-dissertator, the Residence Requirement is a minimum of 8 credits for the fall and spring semesters and 2 credits for the summer semester. As a dissertator, the Residence Requirement is 3 credits each semester. The department encourages each non-dissertator to register for 12 credits in the fall and in the spring in case a course must be dropped.

#### Every Semester

Register for zero credits for Chem. 960

Register for 0-1 credits for Chem. 964 (see timetable; does not apply to the first semester)

#### Non-Dissertator

12 credits in the fall and spring and 2 credits in the summer. Research credits (Chem. 992 or 995) should be used to bring the total to 12. See the timetable for call numbers. The minor agreement form (obtained from the Graduate Program Coordinator in room 2108) should be submitted midway through your coursework.

#### Special notes for the first year:

##### Fall Semester

Enroll in Chem. 661, Chem. 675, Chem. 901 (1 credit), Chem. 960, and 5 credits of Chem. 992 to bring the total to 12 credits. *Note:* when registering for Chem 960 as a 2 credit course, do not list “pchem seminar” on Tuesday at 11:00 AM on your TA schedule card. Instead, list chem. 960 itself – this will avoid scheduling a teaching section during seminar.

##### Spring Semester

Enroll in Chem. 960 as a class for an additional two credits and continue in Chem. 901 (1 credit).

Enroll in Chem. 607 for Laboratory Safety (required, 1 credit)

#### Dissertator

3 research credits each semester (fall, spring, and summer)

Check the timetable for the appropriate class number for your group.

Submit the Request for a Preliminary Warrant form (obtained from the Graduate Program Coordinator) three weeks prior to your ORP defense.

The ORP should be submitted to your evaluation committee at least one week before the defense date.

#### Ph.D. Defense

Submit the Ph. D. Final Oral Committee Approval Form (obtained from

the Graduate Program Coordinator) three weeks prior to your defense. The thesis should be submitted to your evaluation committee at least one week before the defense date.

*Additional Note*

When scheduling the TBO, RP, and Ph. D. defenses, please write the date, time, and location of the defense on the first page of the written document, and remind your committee of this information when you hand them your document and one day in advance of the defense.

### The Blue Schedule Card

**Fall Semester, first year**

Enter: Chem 661 MWF

Chem 675 MWF

Chem 901 (section 1 times)

Research Talks at 5:40 PM, Thursday

Pchem Seminar, 11:00 AM, Tuesday (do NOT enter chem. 960)

Spring Semester, first year

Enter: Chem 960 for 11:00 AM Tuesday along with the other times

Enter Chem 607

Your group meeting times

All other semesters

Enter: Pchem Seminar, not Chem 960, for 11:00 AM Tuesdays. A TA assignment may be scheduled during this time.

All semesters

Do not enter student seminar at 4:30 PM Tuesday. It is too difficult to schedule teaching assignments with this constraint.

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### Graduate Courses in Physical Chemistry

(many of the upper level courses are taught every other year – see the Timetable for scheduling)

**654 Materials Chemistry of Polymers.** 2-3 cr. Polymer classification, synthesis, and molecular architecture; solid state structure and characterization; glassy state and glass transition; polymer rheology in solids and gels; transport, dielectric and optical properties.

**661 Chemical and Statistical Thermodynamics.** 3 cr. Basic chemical thermodynamics with applications to chemical and phase equilibria and the study of solutions; introduction to statistical mechanics and calculation of thermodynamic quantities from molecular models; stability and fluctuations.

**664 Physical Chemistry of Macromolecules.** 2-3 cr. Structure, thermodynamics, and dynamics of polymers in solution and in the bulk; theoretical models and experimental methods; polymer characterization.

**665 Biophysical Chemistry.** 4 cr. Equilibrium thermodynamics, chemical kinetics and

transport properties, with emphasis on solution behavior and application to noncovalent interactions of biological macromolecules in solution.

**675 Introductory Quantum Chemistry.** 3 cr. Basic principles of quantum chemistry, exactly solvable problems, angular momentum, approximation methods, applications to electronic structure.

**762 Molecular Reaction Dynamics.** 2-3 cr. Microscopic approach to chemical dynamics.

**763 Introduction to Molecular Spectroscopy.** 2-3 cr. Quantum mechanics of molecular rotation and vibration; principles of group theory; electronic, vibrational, and magnetic resonance spectroscopy in gas and condensed phases.

**775 Electronic Structure of Molecules.** 2-3 cr. Applications of quantum mechanics to the electronic structure and properties of molecules.

**777 Physical Chemistry of Surfaces.** 2-3 cr. Structure, thermodynamics, kinetics, and reactivity of molecules at the interfaces between gases, liquids, and solids, with applications to catalysis, atmospheric chemistry, monolayers, and thin films.

**860 Selected Topics in Physical Chemistry.** 1-3 cr.

**863 Advanced Molecular Spectroscopy.** 2-3 cr. Advanced quantum mechanical theory of molecular spectra.

**864 Statistical Mechanics.** 2-3 cr. Fundamentals of statistical mechanics; applications to equilibrium and non-equilibrium properties of gases and condensed phases; selected advanced topics.

**869 Physical Chemistry of Proteins and Nucleic Acids.** 3 cr. Current topics in the physical chemistry of biological polymers.

**871 Rheology of Macromolecules.** 2 cr. Linear and non-linear viscoelasticity of polymer systems.

**872 Selected Topics in Macromolecular and Biophysical Chemistry.** 1-3 cr.

**875 Advanced Topics in Quantum Chemistry.** 2-3 cr. Advanced methods and special topics in quantum chemistry.

**960 Seminar—Physical Chemistry.** 0-2 cr.

**962 Seminar—Macromolecular Chemistry.** 0-1 cr.

**964 Seminar—Molecular Dynamics.** 0-1 cr.

**992 Research—Physical Chemistry** 1-12 cr.

**995 Research—Macromolecular Chemistry** 1-12 cr.

## The PhD Program in Chemistry

The requirement to produce a PhD thesis, the dominant feature of any graduate program, unites all doctoral students in Chemistry. Other requirements, however, vary somewhat among the divisions and programs within the Department. The purpose of this document is to suggest a set of guidelines that support a degree of uniformity among these other requirements, while at the same time allowing for the diversity among different programs that is inevitable and desirable in so highly specialized a process as earning the Ph.D.

The key aspect is that the PhD requirements for the *Department* are stated as a sequence of steps, each of which may be completed in *any* division or program. The requirements are represented by six stages: 1) Domain knowledge, 2) Thesis background presentation, 3) Literature evaluation, 4) Research Proposal, 5) Thesis planning meeting, and 6) PhD Thesis. The first four stages will normally be completed before the end of the sixth semester of the student's study. These stages are outlined below, with details determined by each individual program.

### 1) Domain knowledge

The PhD candidate should demonstrate knowledge in a domain of expertise.

Departmental requirements for these skills are normally completed before the end of the *fourth* semester, and it is anticipated that different programs may have different components for this requirement. For example, this requirement could include course-work, completion of a minor, and exams that test domain knowledge skills.

### 2) Thesis background presentation

The PhD candidate should present, justify, and defend the thesis research project.

Departmental requirements for these skills are normally completed before the end of the *fifth* semester. The purpose of this requirement is to assess the student's preparation for research, including the goals, techniques, and background for the problem to be addressed. Actual research results are not required, but may of course be included if available. It is expected that this requirement will include a written and an oral component (your TBO).

### 3) Literature Evaluation

The PhD candidate should demonstrate the ability to read, understand, analyze and critically evaluate research papers.

Departmental requirements for these skills are normally completed between the end of the *2<sup>nd</sup>* and *4<sup>th</sup>* year, and it is anticipated that different programs may have different components for this requirement. Examples include the literature seminars in organic and inorganic chemistry and the series of Topic exams in Physical Chemistry, where (in each exam) students are given a research paper and have to take a written test a week later.

#### **4) Original research proposal**

*The PhD candidate should present and defend an original research proposal*

The original research proposal should be in an area not closely related to the student's PhD research. The proposal should establish that the proposed research will be of interest and that it is feasible. It is expected that the candidate will prepare a written proposal and then present and defend the proposal. It is expected that the entire proposal, including the core idea, its development, and the writing of the document, will be substantially the work of the candidate. The proposal will normally be completed before the end of the 3<sup>rd</sup> year.

#### **5) Thesis planning meeting**

The PhD candidate should present plans for completion of the thesis (mentor committee meeting).

For students who have not set a date for defense of their thesis by the end of the 5<sup>th</sup> year, a thesis committee meeting will be held to review progress, to plan for completion of the PhD research, and to work out an "end-game" strategy. If at this meeting, a thesis completion date within a year is not set, a second meeting will be held six months later. The purpose thesis planning meetings is to help the student make it through the program in a timely manner.

#### **6) PhD Thesis**

The PhD candidate should carry out and disseminate research that goes to the edge of current knowledge and pushes it out a little further.

Scientific excellence is our central goal. This is the final stage, and it is expected the candidate will complete this requirement before the sixth year, although no time constraint is placed.

#### **Thesis committee**

A candidate will have a committee with (at least) three faculty members. The composition of the committee will be decided by mutual consent of the candidate and major professor before the *Thesis background presentation*. The committee will be involved as much as possible in evaluation of each of the requirements.

#### **Philosophy**

All the existing programs and divisions already have the above requirements. The main point of elucidating the structure is that all programs will be more or less *in phase*, i.e., the requirements will occur in sequence and at roughly similar times. This will significantly aid the (admittedly few) students that wish to change programs. A student could, for example, complete the domain knowledge and literature evaluation skills in Physical Chemistry and then complete the rest of the requirements in a different program, without having to repeat any exams.

We also anticipate that this structure will facilitate the creation of new programs. A new

program could be created with requirements taken from existing programs.

We hope that programs will be constructed with “traits of output” in mind, and that successful PhD candidates will:

- Possess domain expertise and breadth of knowledge
- Be self-taught, and able to find, define, and solve new problems
- Possess communication, teamwork, and leadership skills.

## **TOPIC EXAM AND THESIS BACKGROUND EXAM INFORMATION**

### **Topic Exam**

The purpose of the Topic Exams is to gauge, and to help expand, your ability to apply the basic principles of physical chemistry in an integrated fashion to specific situations, and to increase your awareness of applications of these principles in the current literature.

Each Topic Exam will focus on a particular topic or theme, typically associated with one or more papers from the research literature. For example, you may be called upon to demonstrate understanding of the paper, to describe its underlying theoretical or experimental techniques, to solve problems involving such techniques, or to relate the results of the paper to other areas of physical chemistry research. The exam format and the types of questions may vary.

There will be two 3-hour exams, scheduled approximately six weeks apart during the first 12 weeks of the fall semester in your second year. Each exam will be prepared by a different committee of three faculty members. The topic and leading reference(s) will be distributed approximately 10 days before the exam. Examples illustrating the concept of the Topic Exam are on locked-case reserve in the Chemistry Library. Ask for "Topic Exams - Physical Chemistry."

The committee will score its exam on a 5-point scale (5 = excellent, 4 = good, 3 = fair, 2 = poor, 1 = unsatisfactory). For students receiving grades of 3 or lower, and in some other cases, the committee may make individual assignments of follow-up work. Graded exams will be returned.

Within the week following the exam, each student will have a brief conference with a member of the committee to discuss the exam and possibly to receive an assignment and agree on a due date. Assignments will normally be due within one week. The committee will score any assigned work on a 5-point scale.

### **Thesis Background Exam**

The purpose of the Thesis Background Exam is to demonstrate the student's comprehension of the goals, techniques, and background for the thesis research that is to be undertaken.

The exam consists of a written summary and an oral presentation by the student (of approximately 25 minutes duration) outlining the background, aims, and methods of the Ph.D. research that will be pursued, followed by a period of questioning (of about 40 minutes duration) by a committee of three faculty including the research advisor. For example, you may be called upon to answer questions about pertinent background literature, to demonstrate familiarity with some of the techniques which will be required, or to describe the significance of the research and the rationale for the methods to be employed.

The written summary should consist of 1-2 pages, including references, and must be presented to

the committee three days before the oral exam. Please hand deliver your written summary to your committee and send them a copy by email.

The exam will be scored on a 5-point scale. In case of an unsatisfactory performance, the committee may set a date for a second opportunity.

### **Preparation for Exams**

The assumed background for these exams is equivalent to Chem 661, 675, and other physical chemistry graduate courses. Attending and actively participating in seminars and group research discussions, reading the chemical literature, and thinking about the research going on around you, as well as your own research, can all afford valuable experience in relating principles learned in courses to questions of current research interest. In these activities, try to build a broad base rather than concentrating only on areas of greatest immediate interest to you.

While it is true that you must complete these requirements in order to be admitted to candidacy for the Ph.D. degree, their primary purpose is not to screen out students but rather to encourage intellectual activity and growth. Emphasis is placed on providing feedback through face-to-face interactions between students and faculty, and opportunities for special assignments.

### **Review**

After completion of the Topic and Thesis Background Exams, your complete record to date (Exam and Assignment scores, course grades, and research activity) will be reviewed by the faculty of the Physical Division together with major professors not in the Physical Division who have students in the group under review. Possible actions are:

- a) You will be allowed to proceed to the next step in the Ph.D. program.
- b) You will be allowed to proceed, but additional coursework or study in specific areas may be recommended, and you may be required to complete a special assignment.
- c) You will not be permitted to continue in the Ph.D. program. In such cases, an appeal can be made to the Physical Division.

## PRESENTATION OF ORIGINAL RESEARCH PROPOSAL

The purpose of the original research proposal is to provide experience in developing and presenting new ideas for research. The student needs to identify a research goal that is significant and achievable, choose a suitable approach, and describe the major steps and techniques required to reach that goal. A committee consisting of the major professor, as chair, and two other faculty members selected by the major professor evaluates the written proposal and oral presentation. This committee is typically the student's mentor committee, but other faculty members with specific knowledge about the proposal may also be considered.

To begin, the student presents the major professor with one or two suggested research projects and proposed approaches. Upon approval by the major professor, the student develops one of the projects further, preparing a detailed written proposal in a format suggested by the major professor. One week prior to the oral presentation, the student provides a paper copy of the proposal to the committee members and prepares an abstract, with references, that the Physical Chemistry Division secretary distributes to all of the physical chemistry faculty and graduate students. *The abstract should include the time, date, and place of the oral presentation.* Please send a copy by email to your committee as well. All those who are interested are welcome to attend the oral presentation.

The oral presentation should not exceed twenty-five minutes. Following the presentation, a question and discussion period ensues. The first portion of this period includes the audience, but the later portion involves only the student and committee. The committee files a written record of its evaluation of the proposal in the Divisional Office, and the major professor discusses the presentation, proposal, and the committee's evaluation with the student. If the committee finds the initial attempt unsatisfactory, it will provide the student with another opportunity to present a proposal at a later date determined by the major professor in consultation with the committee and student. The committee may request further written material instead of or in addition to a second presentation.

Presentation of the Original Research Proposal represents the last phase of the preliminary examination for the Ph.D. A Preliminary Warrant should be obtained from the Graduate School by visiting the Chemistry Graduate Program Coordinator, Steph Nagle, in room 2108. This takes approximately *three* weeks. Successful completion of the Original Research Proposal requirement will be recorded on the Preliminary Warrant, which should then be returned to the Program Coordinator. The completion of this requirement will also be recorded on the student's record sheet in the Chemistry Graduate Program Coordinator office, room 2108. At this time, the candidate should review all of the information on the record sheet to ensure that it is correct and up to date.

***The student is responsible for preparing the proposal and scheduling the presentation well in advance of the deadline imposed by the graduate school for becoming a dissertator.*** Students may present the proposal in the final two weeks before the deadline ***only under extraordinary circumstances*** and with the explicit approval of their entire committee. Taking the exam just before the deadline leaves too little time for the student to repeat the presentation or provide additional material that the committee might request.