

## 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 path chair.

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

#### *Fall Semester*

- Talks describing 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 five prospective major professors. Major professors are allowed to make commitments beginning November 1. Under normal circumstances, you should choose a major professor no later than November 15. Please submit your research group selection document to April Sonnentag in the physical chemistry path 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 first year 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, if offered.

- You will begin taking additional courses, which are chosen in consultation with 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 **9** 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, leaving a minimum requirement of 2 additional credits in a physical chemistry course. Chem 901, Chem 607 and research credits do not count toward fulfilling the physical chemistry coursework requirement or the minor 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 15 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 path 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 second semester of your second year, you will take a **Thesis Background Oral (TBO)** Exam. This TBO involves a written summary (length depends on your research group) (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 your preparation for research, including the goals, techniques, and background for the problem to be addressed. Preliminary research results are not required, but should 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 our 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 graduate school. 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.
- In the spring of your 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 (format depends on your research group) and an abstract are prepared. The final step of a successful ORP involves a closed oral presentation of 25 minutes or less. The Path Coordinator, April Sonnentag, should be consulted concerning rules and procedures for scheduling ORPs. After successfully completing the ORP contact the Graduate Program Coordinator, Arrietta Clauss, room 2108, to request a warrant to become a dissertator. 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 exactly 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 advisor. It is possible to take a 1-3 credit course and lower the research credits to accommodate the required 3 credit total.

### 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. You will be given a one page form prior to the meeting; fill this out in consultation with your advisor and distribute the completed form to your committee in advance. Please bring hard copies of your CV to the meeting. 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. A Ph.D. warrant must be requested from the Graduate School three weeks before the oral exam; see the Graduate Program Coordinator, Arrietta Clauss, in room 2108 to request the warrant and discuss the other Graduate School requirements to graduate.
- 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 core coursework and minor requirements (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. The Department of Chemistry does not count classes with grades below a B in the minor requirement or the core course requirement, although

theses courses count in the Graduate School GPA.

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

As a non-dissertator, the Graduate School enrollment requirement is 8-15 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 15 credits in the fall and in the spring in case a course must be dropped. Information about courses can be obtained from the on-line Course Guide (formerly known as "The Timetable").

#### Every Semester

Register for zero credits for Chem 960.

Register for 0-1 credits for Chem. 964 (see on-line Course Guide for section number; does not apply to the first semester)

#### Non-Dissertator

15 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 15. See the on-line Course Guide for course 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 (0 credit), and 8 credits of Chem. 992 to bring the total to 15 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 for 1 credit (if offered).

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

##### Dissertator

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

Check the on-line Course Guide for the appropriate class number for your group.

**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, ORP, 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**

Chem 661 MWF

Chem 675 MWF

Chem 901 (Section 1)

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

**Spring Semester, first year**

Chem 960 for 11:00 AM Tuesday and at the other Chem 960 meeting times

Chem 607 (this course occurs during the week prior to the semester)

Your group meeting times

**All other semesters**

Pchem Seminar, not Chem 960, for 11:00 AM Tuesdays; a TA assignment might need to be scheduled during this time.

Your group meeting times

**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 upper level courses are taught every second year – see Course Guide 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 paths 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 paths 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* path. 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 coursework, completion of a minor, and exams that test domain knowledge skills.

#### **2) Thesis Background Oral 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 *fourth* 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 paths may have different components for this requirement. Examples include the literature seminars and the literature assignment in the 2 credit Chem 960 course.

#### **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 paths 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.

## THESIS BACKGROUND EXAM INFORMATION

### Thesis Background Oral Exam

The purpose of the Thesis Background Oral 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 open 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. If the student has obtained preliminary results, these should also be presented. A period of questioning (of about 40 minutes duration) will follow 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 (format depends upon research group) 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 Exam

The assumed background for this exam 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 this requirement 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 Thesis Background Exam, 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, typically the student's mentor committee, evaluates the written proposal and oral presentation. It is important that the chair of the mentor committee and the student's major professor are present for the research proposal.

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 to the Physical Path Coordinator, April Sonnentag. Please include references and *abstract should include the time, date, and place of the oral presentation*. Please send a copy by email to your committee as well. Only your committee will attend your presentation.

The oral presentation should not exceed twenty-five minutes. You may be interrupted with questions during your presentation. Following the closed presentation, a question and discussion period ensues. The committee files a written record of its evaluation of the proposal in the Path 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 may 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, Arrietta Clauss, 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.