

Handbook for Ph. D. Graduate Students

Department of Chemistry

Southern Methodist University

Second Edition, Fall 2012

Overview and Notes

Please bring any mistakes, omissions, typos, to the attention of the Chemistry Department Graduate Director, so we can improve future editions.

This Handbook is intended for use by Ph. D. graduate students in the Department of Chemistry. It details the curriculum and requirements for the Ph. D. degree.

Abbreviations

ORGS: Office of Research and Graduate Studies

OIT: Office of Information Technologies

TA: Teaching Assistant

RA: Research Assistant

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The Admission Process

What happens after you are accepted for admission to the Ph. D. program in chemistry at SMU?

You will receive two offer letters, one from the Office of Research and Graduate Studies (ORGS) and one from the Chemistry Department. The letter from ORGS contains an acceptance form to the Ph. D. Program in Chemistry that you need to sign and return. The letter from the Chemistry Department is an offer of a Teaching Assistantship (TA). This needs to be signed and returned as well. Both acceptance letters can be sent to ORGS.

What happens after SMU receives both acceptances from you?

You will receive a letter from the Office of Information Technologies (OIT) with information about setting up your email account.

Around the beginning of June, you will receive an email from the Chemistry Department Graduate Director welcoming you to the Department. Read this carefully, as it contains important information about your schedule upon arriving at SMU. Note that you need to be on campus about 6 – 7 days before the official start of classes (exact dates are given in the email). During this week, you will take three placement (organic, inorganic, and physical chemistry) examinations, register for classes, get TA assignments, attend the **REQUIRED Teaching Assistant Seminar**, etc.). All details concerning the week prior to classes are given in the email.

Near the end of June, you will receive a letter from ORGS with general information about registration.

Arrival on Campus

When you arrive on campus

Report to the Chemistry Office (Fondren Science, Room 231) at least one-half hour before your first scheduled placement examination. You will be told where to go to take the exam. The Chemistry Graduate Director will be present to answer any questions and to clarify what needs to be done during this week.

The Three Placement Examinations (in organic, inorganic, and physical chemistry)

The results on these examinations will assist in planning your coursework. Placement exams are given to determine the level of the student's background in the fundamental areas of chemistry. **All entering students must take all three exams AT THE SCHEDULED TIMES! Students who fail to take the exams will not be allowed to enter the program.**

Orientation

Orientation takes place the week before classes commence and includes:

1. Meeting with course instructors for specific TA assignments
2. Departmental orientation meeting
3. Teaching Assistant seminar (REQUIRED by the University; otherwise you cannot be paid.)

Registration, etc.

You must register for classes prior to receiving your SMU ID card. You should register after taking the first placement exam. The Graduate Director will advise you on the specific classes. You will also meet with the Graduate Director **after taking all three placement examinations** to determine if any changes to your class schedule are necessary

All registration is done online via the program ACCESS. You will also get payroll setup, obtain your ID card, get a desk assignment, etc.

There is currently a \$50 per semester international student fee at Southern Methodist University.

Brief Overview and Approximate Time Frame for Meeting the Requirements for the Ph. D. Degree in Chemistry

Year 1

- Required course work (9 credit-hours per semester)^(see page 6)
- English as a Second Language (ESL) class for foreign students
- Selection of Research Advisor **by January 10.**
- Initiation of Dissertation research
- Start taking cumulative examinations (“cumes”) at beginning of second semester

Year 2

- Dissertation research
- Completion of cumes
- Presentation of Departmental seminar (Chem 7121) **during the FALL SEMESTER**
- Presentation of Research Synopsis and Objectives (Chem 7233)
(faculty committee must be selected by student and Research Advisor for Chem 7233)

Year 3

- Dissertation research
- Presentation of an original research proposal (Proposal Methodology, Chem 7334)
(faculty committee must be selected by student and Research Advisor for Chem 7334)
- Fill out forms for “Admission to Candidacy”

Subsequent year(s)

- Dissertation research completion
- Completion of required total number of credit-hours (48)
- Oral presentation of research at a professional meeting (Chem 7122)
This can be done at any stage of the student’s research career.
- Prepare and submit Dissertation to Dissertation Committee
Committee must be selected by student and Research Advisor.
- Successful oral defense of Dissertation

Registration Note: Courses that need to be taken with the Research Advisor as the Instructor

Chem 7233, 7334
Chem 7151, 7251, 7351
Chem 7101, 7201, 7301
Chem 7122

When registering, if you do not see your Research Advisor listed as an instructor for any of the above courses, click on VIEW ALL SECTIONS. If your advisor is still not listed, contact the Chemistry Department Administrative Assistant to have your Advisor added to the list of instructors. **Do not register for the class with another faculty member as the instructor.**

******Important Registration Information******

For students WHO HAVE NOT completed the requirements for admission to candidacy:

- Enroll in Chem 6120 or 6121 (Current Topics in Research) each semester.
REGISTER FOR THIS CLASS USING THE NUMBER OF THE DEPARTMENTAL GRADUATE DIRECTOR.
- THE TOTAL OF ALL COURSES **MUST EQUAL 9 HOURS**.
- If your Research Director suggests an additional course, your course load must be adjusted accordingly to fulfill the 9-hour total.

For students WHO HAVE completed the requirements for admission to candidacy:

- Enroll in Chem 8049 each semester.
- THE TOTAL HOURS per term **MUST NOT EXCEED 9 HOURS**. IT CAN BE LESS than 9 hours.
- If you are receiving any type of salary, stipend, etc. (e.g., TA, RA), YOU MUST REGISTER FOR AT LEAST ONE CREDIT HOUR EACH SEMESTER. This is usually Chem 7151 (Research).

Summer Registration: To have access to library and other university privileges, you must be officially registered for a class. You must register for a **credit-bearing class** for several reasons: to receive salary/stipend and health insurance, and for visa purposes. For most students, register for Chem 7151 (Research) with your Research Advisor as the instructor for the entire summer ("Summer 3").

Meeting Presentation (Chem 7122): If you are scheduled to give an oral presentation at a meeting, please register for this class (Fall or Spring semester only, even if presentation is given during summer). Make sure to adjust total hours to 9 **if you have not yet been admitted to candidacy**. Note that this course is taken only once as a Ph. D. student, no matter how many oral presentations are given. Register with your Research Advisor as the instructor.

The number of credit hours for a course is determined by the SECOND digit of the course number. Thus, Chem 7122 is a one-hour course; Chem 7201 is a two-hour course.

Good Standing

A student **must maintain an overall B average** (3.00 on a 4.00 scale) **and receive no more than two grades below the grade of B-**. Failure to meet these requirements will result in either probation and/or dismissal from the graduate program.

The Grade Point Average (GPA) system is the following:

A	4.0 grade points per credit hour
A-	3.7 grade points per credit hour
B+	3.3 grade points per credit hour
B	3.0 grade points per credit hour
B-	2.7 grade points per credit hour
C+	2.3 grade points per credit hour
C	2.0 grade points per credit hour
F	0.0 grade points per credit hour

Graduate Student Progress Reports

At the end of each semester, the Department faculty meets to discuss the progress of all graduate students. Each student then receives a letter from the Graduate Director concerning his/her progress in the program. Enclosed with the letter is a Status Sheet outlining the specific requirements that have been completed and those that need to be completed.

First-Year Required Coursework

(First 1/3, second 1/3, third 1/3 refer to the first, second, and last thirds of the semester)

FALL Track A (All Students)

CHEM 6220	Modern Aspects of Chemistry (first 1/3)
CHEM 6116	Introduction to Bioorganic and Medicinal Chemistry (first 1/3)
CHEM 6115	Theory of the Chemical Bond (second 1/3)
CHEM 6118	Overview of Materials Chemistry (second 1/3)
CHEM 6110	Chemical Communications (last 1/3)
CHEM 6111	Practical Laboratory <u>or</u> Practical Computational Methods (last 1/3)
CHEM 7111	Teaching Practicum I
CHEM 6120	Current Topics in Research

SPRING Track A1 (Organic/Medicinal/Bioorganic Students)

CHEM 5393	Advanced Organic Chemistry
CHEM 6113	Practical Aspects of Spectroscopy (first 1/3)
CHEM 6119	Synthetic Strategies (first 1/3)
CHEM 7251	Research (2 h)
CHEM 7112	Teaching Practicum II
CHEM 6121	Current Topics in Research

SPRING Track A2 (Materials/Polymer Students)

CHEM 5333	Introduction to Polymer Chemistry
CHEM 6113	Practical Aspects of Spectroscopy (first 1/3)
CHEM 6114	Chemical Kinetics (first 1/3)
CHEM 7251	Research (2 h)
CHEM 7112	Teaching Practicum II
CHEM 6121	Current Topics in Research

SPRING Track B (Theoretical/Computational/Physical Students)

CHEM 6343	Computational Chemistry
CHEM 6325	Introduction to ab initio calculations: Hartree-Fock
CHEM 7151	Research
CHEM 7112	Teaching Practicum II
CHEM 6121	Current Topics in Research

Requirements for the Ph. D. degree in Chemistry – More Details

Part 1. Requirements for “Admission to Candidacy” (usually completed in the third year)

Research Director must be selected by **January 10 of the first year**

CHEM 6220 Modern Aspects of Chemistry is taken by all entering Ph. D students. This course is offered during the first third of the entering semester. Each faculty member provides an overview of their research in this course to familiarize all entering students with the research being conducted in the Department.

The student must complete all required courses. (see page 6)

Teaching Practicum (Chem 7111 and 7112)

Each student must complete both semesters of this course, usually in the first year. This course is critical for Ph. D students to develop teaching skills needed throughout their career. Hence, each student's performance is monitored carefully and students turn in written projects. The duties involve 10 to 25 hours of lab, lecture, proctoring, grading, etc. each week. Details of this course are provided in the section on Teaching Practicum in the Appendix. These courses are taken each semester that the student is a Teaching Assistant.

Current Topics in Research (Chem 6120 and 6121) SEMINAR

Each student must **complete at least four semesters** of this course. **Prior to Admission to Candidacy, each student will register for Chem 6120 or 6121 each semester.** This includes **mandatory attendance at all Departmental seminars**, whether given by outside speakers or from within the Department. Missing more than two seminars a semester will constitute a failing grade. Each student is responsible for clearing absences with the faculty member in charge of Chem 6120 or 6121 for that semester. A seminar calendar is located on the Department website, and should be consulted frequently since there are likely to be changes throughout the semester.

Cumulative Examinations (cumes)

The purpose of the cumulative examinations is to aid students in developing a thorough understanding of both fundamentals of and recent advances in chemistry.

Each student takes cumulative exams (cumes) until the required total score of 25 is obtained. A maximum of 12 cumes can be taken. Each cume is graded on a zero to 5 point scale. Students begin taking cumes during the spring semester of their first year. Eight cumes are given per year and are usually scheduled during the last week of August, September, October, November, January, February, March, and April. Once students begin taking the cumes, they are required to continue taking them in sequence. Thus, a student taking his/her first cume in January completes the twelve in April of the following year, regardless of whether or not they miss an exam.

Track A1 (Organic/Medicinal/Bioorganic) and Track A2 (Materials/Polymer) Students

Students are given a choice of two different exams and decide which one to take after looking over both at the beginning of the exam period.

Track B (Theoretical/Computational/Physical) Students

Students get details from the faculty member writing the exam.

Departmental seminar (Chem 7121)

Each student presents a 45- to 50-minute seminar to the Department on a current topic in chemistry. The topic must be unrelated to the student's own dissertation research. The course is graded on an A, B, C basis by the faculty present at the seminar. **Details are provided in the Appendix.**

Research Synopsis and Objectives (Chem 7233)

Each student writes a report of research progress and future research directions. The student gives an oral presentation to the Department on this report and defends this in front of a faculty committee. The course is graded on a P/F basis by the committee. **Details are provided in the Appendix.**

Proposal Methodology (Chem 7334)

Each student develops an original research idea and writes a proposal based on this work. The topic must be unrelated to the student's own dissertation research. This proposal is presented to the Department, and the proposal is defended by the student in front of a faculty committee.. The course is graded on a P/F basis by the committee. **Details are provided in the Appendix.**

Admission to Candidacy Procedure

After completion of the above requirements, the Ph. D candidate is eligible for Admission to Candidacy. Admission to Candidacy involves filling out [several forms](#) from the ORGS office (ORGS-Form 1, pages 1, 2, and 3). See Graduate Director for details.

Part 2. Final Requirements for the Ph. D. Degree

Meeting Presentation (Chem 7122)

Each student is required to give an oral presentation of his/her research at a professional meeting of chemists or chemical scientists, e.g., a national, regional, or local meeting of the American Chemical Society (ACS). *This can be accomplished at any stage of their research career. Completion of Admission to Candidacy requirements is not needed.*

The Dallas-Fort Worth section of the ACS hosts the annual Meeting-in-Miniature every April. These are held at neighboring universities and there are sessions for graduate student presentations. This is an excellent opportunity for students to fulfill this requirement and it is strongly advised that each student do a presentation more than one year during the Ph. D. program, since practice giving presentations and answering questions is a vital skill for the professional chemist.

Completion of the 48-hour requirement of graduate credit

Successfully write and orally defend Dissertation

This is the final Ph. D. defense. The written Dissertation on a substantive body of research is presented to a faculty committee and orally defended in front of this committee. The faculty committee consists of the student's research director, three faculty members (usually from the Department), and one faculty member from outside the Department as required by the ORGS.

Scheduling Presentations, Proposals, and the Final Defense

Scheduling should be done in consultation with the Graduate Director for the semester and with the student's committee members. The student committee must be available at this time and date. Once this is worked out informally, **it is the student's responsibility to give the committee the time and date, in writing. This should be done no less than three weeks prior to the date of the presentation or defense.** The student should be aware that it is often more difficult to assemble the committee during the summer.

Dissertation and Final Defense

Prior to scheduling the dissertation defense, the student should respectfully invite a faculty member from outside the Department of Chemistry to serve on the Dissertation Committee. This person is usually selected after consultation with the student's research director. In some cases, the student may petition to have a faculty member from another university serve on the committee if that person has special expertise in the student's area of research. Prior approval of the Dean of Dedman College is required for committee members from another university. The remaining four members of the committee to whom the student defended the earlier proposals and research (Chem 7233 and 7344) may also serve on the Dissertation Committee.

The Dissertation Topic Report (ORGS Form 2) needs to be filled out by the Ph. D. candidate and brought to ORGS as soon as the Dissertation Committee has been selected.

The Ph. D. Examination Report Form (ORGS Form 3) must be filled out by the Ph. D. candidate and signed by the Dissertation Committee when the candidate passes the defense.

Scheduling of the final defense should be done in consultation with the faculty seminar coordinator for the semester and with the student's committee members. The student committee must be available at this time and date. Once this is worked out informally, **it is the student's responsibility to give the committee the time and date, in writing. This should be done no less than three weeks prior to the date of the presentation or defense.** The student should be aware that it is often more difficult to assemble the committee during the summer.

The student is expected to adhere to the Office of Graduate Studies and Research required dissertation format and to work closely with the personnel in that office. Once the dissertation is completed, the "[Thesis Release Form](#)" should be completed and submitted along with the thesis.

Finally, the student must also complete an "[Application for Candidacy to Graduate](#)" form. <http://smu.edu/graduate/files/ACG.pdf>.

The student should review all University deadlines carefully well in advance of the final defense at <http://smu.edu/graduate/deadlines.asp>. This will avoid being "caught by surprise" by these deadlines. For example, the "Application for Candidacy to Graduate" form is due in January for the following May graduation.

Annual Research Day NEW 2012 – 2013 academic year

Ph. D. students give oral presentations on their research.

In a competitive job market, any skill that distinguishes you from other candidates is essential for acquiring a top tier position. The ability to orally present research information in a concise and complete manner is required for both industrial and academic positions. Moreover, the ability to work in a team environment that incorporates multiple scientific disciplines is a hallmark of the modern research environment.

To better prepare Chemistry Ph.D. students, we have established an **Annual Research Day**. This environment will help hone presentation skills and allow you to show your peers the work you have accomplished. Familiarizing yourself with each others' work and critiquing the scientific aspects of your progress also exposes each student to new disciplines and techniques.

Annual Research Day format:

- Ph. D. Chemistry students present 30-minute talks on their research to all Ph. D. students in the Department.
- Student oral presentations begin in their second year and continue until graduation.
- All Ph D students are required to attend.

APPENDIX

Chemistry (CHEM) Graduate Courses

5185. Laboratory Methods in Physical Chemistry. Laboratory experiments with emphasis on thermodynamics, chemical kinetics and physical biochemistry. One half-hour of lecture and five-hour laboratory period each week for five weeks. *Prerequisite:* CHEM 5381 or 5383.

5188. Advanced Physical Chemistry Laboratory. Laboratory experiments with emphasis on chemical kinetics and molecular spectroscopy. One half-hour of lecture and five-hour laboratory period each week for five weeks. *Prerequisite:* CHEM 5185. *Corequisite:* CHEM 5384 or permission of the instructor.

5192. Inorganic Chemistry Laboratory. Synthesis and characterization of transition metal and main group element compounds and solid-state materials. *Prerequisite or Corequisite:* CHEM 5392.

5306. Computational Chemistry. Introduction to the techniques of computer modeling of small to medium-sized organic molecules using advanced graphics workstations. *Prerequisite:* CHEM 3372.

5310. Biological Chemistry: Macromolecular Structure and Function. Introduction to the structure and function of macromolecules of biological importance. Emphasis on nucleic acid and protein structure, enzyme kinetics, and carbohydrate and lipid chemistry. Three lecture hours per week. *Prerequisites:* CHEM 3371 (3373) and 3117 (3119).

5311. Metabolism. Introduction to the pathways and regulatory events in the metabolism of carbohydrates, lipids, amino acids and nucleotides. Three lecture hours per week. *Prerequisites:* CHEM 3371, 3372.

5312. Physical Biochemistry. Physical chemistry of macromolecules and biological membranes, with an emphasis on the thermodynamics of solutions. *Prerequisites:* MATH 1338 and CHEM 3372, 5310. (CHEM 5381 or 5383 recommended)

5317. Introduction to Molecular Modeling and Computer Assisted Drug Design. The course presents a thorough and in depth overview of methods and techniques in computer assisted drug design (CADD). It includes topics such as drug discovery and drug design, molecular recognition and docking, ligand-receptor interactions, pharmacophore searching, virtual screening, de novo design, molecular graphics, chemometrics, etc. *Prerequisite:* Permission of the instructor.

5321. Understanding Chemistry. The course focuses on a general understanding of chemistry in terms of models and concepts that describe structure, stability, reactivity and other properties of molecules in a simple, yet very effective way. *Prerequisite:* Permission of the instructor.

5322. Introduction to Nanotechnology. Nanotechnology (NT) is expected to change our lives and society more than computer technology and electricity have done together. The course will provide an introduction to NT. Nano-materials and their applications will be discussed. *Prerequisite:* Permission of the instructor.

5333. Introduction to Polymer Chemistry. Provides an introduction to the synthesis, physical properties and solution properties of high molecular weight molecules. Plastics, manufacturing and fabrication of polymers.

5335. Advanced Laboratory Methods and Techniques. Advanced techniques and methods in the synthesis of chemical compounds.

5383. Physical Chemistry I. Gas laws, elementary kinetic theory and the four laws of thermodynamics, including applications to phase diagrams and biological processes. *Prerequisites:* PHYS 1106, 1304 (or 1408) and MATH 2338. *Prerequisite or Corequisite:* CHEM 3351.

5384. Physical Chemistry II. Elements of quantum mechanics and its description of many electron atoms, bonding and spectroscopy, intermolecular forces, structure of solids, chemical kinetics, and transport properties of fluids. *Prerequisite:* CHEM 5383.

5387. Thermodynamics and Statistical Mechanics of Materials and Solid State Reactions. Examines the relationship between partition function and thermodynamic variables. Derives transport properties from random-walk models and kinetic theory. Studies solid-state reactions, transport at interfaces, phase transformations and nucleation using techniques from both microscopic and macroscopic theories.

5390. Environmental Chemistry. An examination of the chemistry of earth's environment, with emphasis on problems caused by human activity. Includes aquatic and soil chemistry, nuclear chemistry, combustion, alternative energy technologies, atmospheric chemistry, and global warming. *Prerequisites:* MATH 1338, PHYS 1303 or 1407, and CHEM 1304. *Recommended:* PHYS 1304 or 1408, CHEM 5381 or 5383, or GEOL 6338.

5392. Advanced Inorganic Chemistry. Survey of the bonding, structure and reactivity of inorganic compounds. Coordination, organometallic and main group element chemistry. Three hours of lecture each week. *Prerequisite:* CHEM 5384.

5393. Advanced Organic Chemistry. Three hours of lecture per week. *Prerequisite:* CHEM 3372.

5395. Advanced Analytical Chemistry. Three hours of lecture each week. *Prerequisite:* CHEM 5486.

5396. Advanced Physical Chemistry. Three hours of lecture each week. *Prerequisite:* CHEM 5384.

5397. Biotransformations and Biocatalysis. Covers the history, application and current trends of biotransformations and biocatalysis with emphasis on how biocatalysts are developed and used in pharmaceutical research.

5398. Medicinal Chemistry. Emphasizes the design, mode of action and metabolism of drugs, including antibiotics, antifungals, antivirals, anticancer agents, CNS agents and analgesics/anti-inflammatory agents. *Prerequisites:* CHEM 3371, 3372.

5486. Instrumental Analysis. The theory, operation and application of instrumentation used in the modern chemical laboratory. Two hours of lecture and two three-hour laboratory periods each week.

6000. Research. For students who hold fellowships, but are not enrolled in any credit-hour courses. No tuition.

6049. M.S. Graduate Full-Time Status.

6110. Chemical Communications: Literature, Writing and Presentations. Fundamentals of literature searching, scientific writing, oral and poster presentations, and research notebooks.

6111. Practical Laboratory Methods. Describes the theory behind and practice of laboratory techniques necessary to perform advanced synthetic chemical research.

6112. Advanced Stereochemistry. Advanced study in molecular geometry and relationships in space between atoms and groups in a molecule.

6113. Practical Aspects of Spectroscopy. Basic theory and practical applications of spectroscopy for chemists.

6114. Chemical Kinetics. Kinetics of gas-phase, surface, condensed-phase, polymer, photochemical and enzyme reactions.

6115. Theory of the Chemical Bond. Covers different descriptions of covalent bonding, including the ability to predict bonding structures in molecules and methods to test these predictions.

6116. Introduction to Bioorganic and Medicinal Chemistry. Protein structure, enzymes and receptors as drug targets, enzyme inhibitors, design of agonists, and design of antagonists.
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6117. Chemical Periodicity: Reactivity and Structural Trends in Inorganic and Organometallic Compounds. Explores periodic or recurring trends of the chemical elements in terms of their properties and chemical behavior.

6118. Overview of Materials Chemistry. Surveys the synthesis, characterization and applications of ceramics and glasses, polymers, metals, nanomaterials, semiconductors and conductors, and biomaterials.

6119. Synthetic Strategies. Formation of the carbon skeleton, organometallic reagents and coupling reactions, protecting groups and chemical compatibility, and convergent synthesis.

6120, 6121. Current Topics in Research. Review of current research as presented by visiting lecturers.

6130. Mechanisms in Organic, Organometallic and Bioorganic Chemistry. Fundamental mechanistic concepts in bioorganic, materials, medicinal, organic and organometallic chemistry. Emphasizes mechanistic similarities of seemingly different types of reactions.

6220. Modern Aspects of Chemistry. Overview of current important topics in chemistry and the relationship to research programs in the department. *Prerequisite:* Official admission to graduate program.

6306. Computational Chemistry. An introduction to the techniques of computer modeling of small to medium-sized organic molecules using advanced graphics workstations. *Prerequisite:* CHEM 3372.

6308. Special Topics in Chemistry. Presentation of advanced special topics that are at the forefront of current chemical interest. Content varies from term to term.

6302. The Chemical Bond.

6312. Theory of Organic Chemistry.

6325. Introduction to ab initio Calculations: Hartree Fock Theory. Quantum chemical investigations of the ab initio type normally start with a Hartree-Fock calculation. Students interested in quantum or computational chemistry have to acquire basic knowledge in Hartree-Fock theory before starting with the more advanced electron correlation theories. This course provides an introduction into Hartree-Fock theory. *Prerequisite:* Permission of the instructor.

6331. Theory of Analytical Chemistry.

6341. Advanced Models and Concepts in Chemistry. Advanced models and concepts will be presented to understand the structure, stability, and reactivity of molecules in organic, inorganic, and polymer chemistry. *Prerequisite:* Permission of the instructor.

6342. Nanotechnology – Fundamentals and Applications. Nanotechnology (NT) is an interdisciplinary field including among other Nanosciences, Nanoengineering, and Nanomedicine. The course will provide the fundamentals and present applications of nanotechnology in a variety of different disciplines. *Prerequisite:* Permission of the instructor.

6343. Advanced Computational Chemistry. The present course will provide an in-depth training on how to use the computer as a modern efficient tool to solve chemical problems. Major quantum chemical packages will be used. Prerequisites: The course is designed for all graduate students from chemistry, biochemistry, medicinal chemistry, biology, and engineering who want to obtain a thorough and in-depth overview over methods and techniques applied in computational chemistry. Since the course addresses a broad audience, it is designed as an interdisciplinary course taking care of the special needs of graduate students with different backgrounds. *Prerequisite:* Permission of the instructor.

6344. Computer Assisted Drug Design – Fundamentals and Applications. The course discusses the fundamentals of computer assisted drug design (CADD), the latest and important developments in CADD methodologies, and their applications. Topics stretch from drug discovery over virtual screening, to de novo design and neural networks, etc. *Prerequisite:* Permission of the instructor.

6351, 6352. Methods and Techniques of Research.

6397. Biotransformations and Biocatalysis. Covers the history, application and current trends of biotransformations and biocatalysis with emphasis on how biocatalysts are developed and used in pharmaceutical research.

6398, 6399. Thesis.

7101, 7201, 7301. Advanced Independent Study. Readings in the chemical literature on current research topics related to the student's area of research.

7108, 7208, 7308. Special Topics. Presentations of contemporary topics in chemistry.

7111, 7112. Teaching Practicum. Discussion and experience in teaching and communication in the laboratory and classroom.

7121. Departmental Presentation. Major presentation to the entire department on a topic developed from the literature.

7122. Meeting Presentation. Oral presentation at a professional meeting.

7151, 7251, 7351. Research.

7233. Research Synopsis and Objectives. A written report of research progress and development of a written research plan for the Ph.D. research program. Must be defended before a faculty committee.

7334. Proposal Methodology. Development of a written research proposal that is defended before a faculty committee.

8049. Ph.D. Graduate Full-Time Status.

8698, 8699. Dissertation.

Chem 7121

Departmental Presentation

Preparation time for this course is to be in addition to the student's usual research, TA, etc. duties, not a substitution for these duties.

Objectives

The overall objective of all presentations is to expand the student's communication skills and to provide guidance and experience in selecting, organizing, and formally presenting technical information. The Departmental Presentation is to be made on a topic developed from extensive literature research on a subject of current interest. In addition, this presentation should supplement the graduate curriculum with discussions of important, current subjects that are not covered in the traditional courses.

Choice of Topics for Departmental Seminar

Requirements. The main content of the Departmental Seminar must be based on several papers (not a single review article) from the recent literature (i.e., articles published within the last five years). The topic cannot be related to any of the student's present or past research. It cannot be directly related to any courses that the student is taking or to any seminars that the student has given at SMU or elsewhere.

Other Considerations. Topic selection should be of broad, general interest since the audience will be from various disciplines within chemistry. The introduction (which may be based on review articles, books, or other general sources) must explain the overall significance of the subject -- i.e., **why is it important and interesting?** The content of the seminar should be as multi-dimensional and varied as possible. For example, it might include information about the synthesis, structure, reaction mechanisms, applications, etc. of an interesting new class of compounds. Presentations with slide after slide of similar reactions, structures, mathematical equations, etc. are easy to do, but they become very tiresome to the listener and have little educational value.

Procedures for Presentations

- select a topic that is approved by the instructor for Chem 7121 and the student's research advisor. The subject should not be directly related to the student's research project and the student will be encouraged to choose a topic in a completely unrelated field to broaden their general knowledge of chemistry.
- provide a detailed outline to the Chem 7121 instructor at least three weeks prior to the presentation. This will include a bibliography and should not be solely based on a single review article.
- write an abstract which must be approved by the instructor. This should be done no later than two weeks before the presentation.
- prepare all presentation material (e.g., PowerPoint). At least **one week** before the seminar date, submit your complete electronic presentation to the instructor for final approval.
- practice the presentation before other graduate students and before the student's research advisor.
- prepare, distribute, and post flyers announcing the seminar and send email announcement to all department members five days before the presentation
- make a 45 to 50 minute presentation before all the faculty, students, and research associates in the department as part of the departmental seminar program
- answer questions from the audience at the end of the presentation

Presentation

An organized, professional style presentation is required. The individual slides must be carefully prepared and easily readable from the rear of the room (check it out!). Each slide should contain only one key piece of information (e.g., one reaction, one structure, one equation, or a **short** list of bullet points). Long tables of data and paragraphs of text are generally useless and only serve to irritate the audience. The speaker's job is to inform the audience and teach about your topic, not merely to read the slides. Excellent information on oral presentations may be found in the *ACS Style Guide*.

Abstract

A brief, but informative, abstract (one page, double-spaced) of your talk with an accompanying list of references is required. Once approved by the instructor, this must be distributed as described above. The style of the abstract, including the format of the references, should follow standard ACS guidelines (consult the ACS Style Guide and formats used in recent ACS journals). **References should be numbered in sequence and should refer to specific statements in the abstract.**

Advice

Practice, practice, practice! Do not just sit and think about your talk or say it to yourself. Practice it out loud to yourself many times and at least twice (with the slides) to a small group, **including your research director**. Do this at least a week in advance so that you will have time to incorporate their suggestions into your final presentation. Above all, **make sure that your introduction and conclusion are very smooth** since these are the parts to which most people will pay the closest attention. The complete seminar should be **45 - 50 minutes** in length. A short presentation indicates a lack of preparation and will result in a grade of "no credit" for the seminar.

Evaluation

The Departmental Seminar will be graded with a letter (A, B...) grade. The final grade is assigned by the instructor who will solicit written comments and numerical scores from the faculty in attendance (see attached score sheet). An informal "peer" evaluation by the graduate students in attendance will also be conducted after the seminar.

Schedule

- At least **three weeks** before the seminar date, have your topic approved - first by your research advisor, and then by the instructor.
- At least **two weeks** before the seminar date, a typed draft of your abstract (including references) must be submitted to and approved by the seminar coordinator.
- At least **one week** before the seminar date, electronically submit your complete presentation to the seminar coordinator for final approval.
- **Two days** before the seminar date, distribute your abstract (proofread it again!) to all faculty, students, and postdocs.

Failure to meet these deadlines will result in a grade of No Credit for the seminar. The entire seminar process, generally on a new topic, must then be repeated as soon as possible.

Attendance

All graduate students (not just those scheduled to speak) are expected to attend all of the seminars including those given by SMU students as well as by visiting speakers. Also, all students are expected to actively participate in the question and answer period following the seminar.

Chemistry Seminar Evaluation Form

Speaker _____ Date _____

	Poor (1 pt)	Fair (2 pts)	Good (3 pts)	Excellent (4 pts)
Choice of Topic				
Knowledge of Subject				
Organization of Presentation				
Style of Presentation				
Timing of Presentation				
Quality of Visual Aids				
Answering questions				
Abstract				
Total Points				

Additional Comments:

Please write your useful, constructive comments on the BACK of THIS PAGE. The goal is to help this student give better presentations in the future. By writing comments on the back of this page, we will be able to photocopy your evaluation grid to give to the student, but your comments will remain anonymous. We will type the comments as a bullet point list and send these to the student separately.)

Signature (Faculty only) _____ Letter Grade _____ (A, B, C....)

Chem 7233

Research Synopsis and Objectives

Preparation time for this course is to be in addition to the student's usual research, TA, etc. duties, not a substitution for these duties.

(Register for the section listing your research advisor as instructor.)

Objectives

This is a written report of research progress and future research plans for the Ph. D. program that is defended before a faculty committee, usually the same committee that will ultimately serve as the student's dissertation committee. The specific objectives are to present current research results of the student's research and to outline a plan for the dissertation research with a clear understanding of prior work and literature precedence for the proposed work.

Procedures

The student will

- a. write a paper -- the Progress Report and the Prospectus of Research -- detailing current research results and a plan of the proposed work that is needed to complete a dissertation. A significant portion of the document should be dedicated to extensive literature information to justify the proposed work. An electronic copy of the paper should be submitted to the committee members **at least 7 days in advance** of the scheduled oral presentation date. Check with each committee member to see if a hard copy is also needed.
- b. make an oral presentation to the department based on the written report.

Evaluation

- a. The paper will be read by the faculty committee and the presentation will be made to the whole department.
- b. The faculty committee will meet with the student after the departmental presentation for additional questions about both the Progress Report and future work.
- c. The committee will
 - i. determine if the student is making satisfactory progress,
 - ii. determine if the student has demonstrated strong commitment, enthusiasm, and diligence toward completing the degree,
 - iii. determine if the student has demonstrated significant knowledge of the research project and understanding of the related literature,
 - iv. determine if the student has received adequate supervision and guidance from his/her faculty advisor,
 - v. determine if the student has a project with the depth and scope sufficient for the Ph. D. degree,
 - vi. make suggestions for the proposed research.
- d. Acceptance of the presentation and paper will be indicated by the committee members signing the Approval Page (see sample at end of this document) following the discussion period after the presentation.

- e. A grade of Pass or Fail will be assigned based on the presentation and paper (in its original state) at the end of the semester. Additionally, if any committee member does not approve of the paper (indicated by withholding their signature), a grade of Incomplete will be assigned for the class until any requested changes or additions are made. Therefore, any modifications requested by the committee members should generally be completed before the end of the semester in which the course is taken. As a condition of committee approval, all students are expected to demonstrate proficiency in written and spoken English. If proficiency is not demonstrated, additional English as a Second Language (ESL) classes may be required.

Frequently Asked Questions:

1. When is this course taken?

Usually, during the fourth regular semester (summers are not counted) of the student's residency in the program.

2. How is the faculty committee chosen?

The faculty committee should be chosen by the student in consultation with his/her research director. Generally, faculty with expertise closely related to the student's research should be selected. The same committee will usually serve as the committee for Chem 7334 and as the dissertation defense committee.

3. What is the appropriate size of the faculty committee?

The committee is comprised of student's faculty advisor and 3 other faculty from within the chemistry department. In some cases a fourth (full-time, tenured or tenure track) faculty member from a department (e.g., biology) with appropriate expertise in the student's project should also be included as advised by the research director. **NOTE:** For the final Dissertation defense committee, one member must be chosen from another science department. This information is also found in the Graduate Catalog.

4. What is the appropriate length of the written document?

There are no definite length guidelines for the Progress Report and Prospectus of Research, since the nature of the research accomplished and proposed work will vary with projects. Generally, 15 to 20 pages, double-spaced should be appropriate, excluding experimental data which might best be included in an Appendix.

5. What format is followed for the written paper and departmental presentation?

The ACS format for references is required for the written paper and presentation. Students should refer to the *ACS Style Guide* for instruction on proper scientific writing and presentation. The report should have the following format:

- a. Abstract – brief informative overview for distribution to the Department prior to the oral defense
- b. Introduction – background, significance, goals
- c. Research Results – summary of results obtained by the time of writing
- d. Future Directions – description of plans and goals
- e. Experimental Section – journal style format of experiments conducted to date
- f. Literature citations (ACS Style)

All pages must be numbered consecutively.

6. When is the paper due and to whom is it distributed?

The paper must be given to the faculty committee members at least **7 days** in advance of the scheduled presentation. Check with each committee member to determine if he/she prefers an electronic or hard copy.

7. How is the presentation scheduled?

Scheduling should be done in consultation with the research advisor.

8. What is the appropriate length (time) of the oral presentation to the department?

A typical length is between 40 and 50 minutes with a period for answering questions from the general audience. Schedule a room for a longer period to provide time to meet with the faculty committee.

Helpful tips

- i. The Progress Report and the Prospectus of Research should cover all major research projects that the student is conducting and plans to conduct during the dissertation research.
- ii. Comprehensive literature research is essential in order to know how your work significantly advances science. All relevant literature directly related to your proposed research should be mentioned and referenced as evidence of your thorough knowledge in the area. Use the effort required to prepare your presentation and paper as an opportunity to become an expert in your area.
- iii. Pay extra attention to interesting areas such as failed reactions and unexpected results. Try to give scientific explanations for such results. Another purpose of the progress report is to gauge your scientific expertise and maturity in the area of your research.
- iv. Ask a colleague to take notes during the question/answer session of the presentation. Questions raised during this presentation are likely to resurface during the thesis defense.
- v. Make things clear to the reader who DOES NOT KNOW AS MUCH as you do. It is far better to over explain than not be clear. The last thing you want to do is irritate the reader by making him/her look up things. Make it UNDERSTANDABLE!
- vi. Allow PLENTY of time to complete the paper and to prepare for the presentation. Everything will take 3 to 5 times longer than you think.

Sample Approval Page: Student must prepare this page prior to presentation and give it to the faculty committee at the presentation.

(Allow 2" top margin)

THE TITLE IS IN ALL CAPS, NO MORE THAN 48 CHARACTERS SPACES
TO A LINE, CENTERED BETWEEN MARGINS, DOUBLE SPACED
ARRANGED IN AN INVERTED PYRAMID SHAPE

Chemistry 7233 – Research Synopsis and Objectives

Student Name

Date of presentation (*italics*)

Approved by: (Allow adequate space for signatures)

Single space name & title below line

List in order of Advisor, others alpha order

List in order of Advisor, others alpha order

List in order of Advisor, others alpha order

Fourth line only if committee member from outside of
Chemistry Department is included

CHEM 7334

Proposal Methodology

Preparation time for this course is to be in addition to the student's usual research, TA, etc. duties, not a substitution for these duties.

(Register for the section listing your research advisor as instructor.)

Objectives

The primary objective is to develop the student's creativity and critical thinking by conceiving and fully developing an original research idea. The student will write a proposal describing the idea and plans for implementing the research and will defend the proposal before a faculty committee. The proposal topic must be unrelated to the student's dissertation research topic. The student will be judged on the novelty of the idea and the development of a sound and feasible method of investigation.

Procedures

Based on extensive reading of the literature the student will select and develop a research project addressing **a problem that has not been solved** and that is **unrelated** to the student's Ph. D. research or other work in his/her research group. The subject must be approved by the student's research director and the Graduate Advisor. Since this is an original research proposal, the research director may provide only minimal guidance on topic selection and will not proofread the document prior to submission to the entire committee.

- a. The written proposal will be in the style of a National Science Foundation (NSF) proposal with the following sections: Project Summary, Background, Proposed Work, Broader Impacts, Proposal Budget (using SMU fringe benefit and overhead rates), Budget Justification, and References. The NSF *Grant Proposal Guide* is available online and is useful for general guidelines, including budget items. See the *Content* section of the Guide for further explanation of broader impacts. All references should be done using standard ACS format. An electronic copy of the proposal should be submitted to the committee members **at least 7 days in advance** of the scheduled oral presentation date. Check with each committee member to see if a hard copy is also needed.
- b. The student will make a 15 minute oral presentation briefly giving the basis for the work and outlining the project. This presentation will be made before the entire Department. This will be followed with questioning by the committee.
- c. Proposal ideas arise from reading the current literature, broad topical material such as C&E News, review articles, and discussion with others. Although the student's research director cannot provide the idea, it is wise to run this past him or her before spending significant amounts of time. It is strongly advised that the proposed project is kept narrow and focused, and therefore manageable.

Timeline

- a. One week prior to the presentation, the student should submit the completed proposal to the each faculty committee member. Five days before the presentation, an announcement should be sent to the Department that includes the title of the proposal.
- b. It is the student's responsibility to
 - set up and confirm the exam date with each committee member
 - reserve a room to meet with the committee (usually for two hours)

- provide the form for signatures (see end of this document) at the time of the exam or after conditions are met
 - meet with the Graduate Director after successfully completing this class to submit required ORGS forms for Admission to Candidacy
- c. All conditions for a "Conditional Pass" must be met by the deadline decided by the faculty committee. (See below)

Evaluation

- a. The committee will determine if
- i. the project goals are clearly delineated.
 - ii. the project would advance "knowledge and understanding within its own field or across different fields".
 - iii. the project develops a sound and feasible method of achieving the proposal objectives
 - iv. the project is "well-conceived and organized".
 - v. the project could "benefit society".
- b. Based on the written proposal, the presentation, and the student's ability to answer questions, one of the following grades will be given by the committee.
- i. Pass. The student proceeds in the Ph. D. program. This is generally the last formal requirement before the student is admitted to candidacy.
 - ii. Conditional Pass: The student will be required to complete a set of requirements (e.g., rewriting the proposal, meeting again with the committee, repeating the exam completely including a second proposal, completing additional coursework to fulfill deficiencies in knowledge, etc.) The condition(s) and the time-frame for completion must be precisely described in writing and provided to the student as soon as possible, preferably before the end of the day of the exam. A copy of these written conditions must also be provided to the Graduate Director.
 - iii. Fail: The student is not allowed to pursue the Ph. D. program and is encouraged to work toward an M.S. degree.
- c. Acceptance of the Proposal and Presentation will be indicated by the committee members signing the Approval Page (see form at the end of this document) following the discussion period after the presentation.

Frequently Asked Questions:

1. When is this course taken?

Usually, during the fifth regular semester (summers are not counted) of the student's residency in the program.

2. How is the faculty committee chosen?

The faculty committee is usually the same committee* who evaluated the student in Chem 7233.

*The committee is comprised of student's faculty advisor and 3 other faculty from within the chemistry department. In some cases a fourth faculty member from a department (e.g., biology) with appropriate expertise in the student's project should also be included as advised by the research director. **NOTE:** For the final thesis defense, a fifth member is always chosen from another science department. This information is shown in the Graduate Catalog.

3. What is the appropriate length of the written proposal?

Generally, 15 to 20 pages, double-spaced should be appropriate.

4. How is the presentation scheduled?

Scheduling should be done in consultation with the faculty members on the committee.

Helpful tips

- a. Make sure to keep your topic focused and manageable. Topics that are too broad can lead to a conditional pass.
- b. Comprehensive literature research is essential in order to conceive a sound idea that will significantly advance science. Look for an area that interests you, read all you can find, and then think about questions that remain in the field. Then shape your proposal around those questions and information that is needed to advance the field. All relevant literature directly related to the proposed research should be mentioned and referenced as evidence of your thorough knowledge in the area. Use the effort required to prepare your presentation and paper as an opportunity to truly become an expert in a **new** area.
- c. Your idea should be a significant advancement in your chosen area. Incremental improvements on previous findings may not be deemed significant.
- d. The best proposals offer more than one method to achieve the goals. For example, at least two feasible syntheses of target molecules should be given. Have a backup plan for everything.
- e. It is often best to bullet point the objectives and then shape the proposal sections around these objectives.
- f. Spend extra time on the abstract and make sure the objectives are clearly listed in the abstract.
- g. In addition to a cover page, also include a Table of Contents
- h. Put page numbers on each page and ask each committee member if they prefer a hardcopy or an electronic copy.
- i. Make things clear to the reader who DOES NOT KNOW AS MUCH as you do. It is far better to over explain than not be clear. The last thing you want to do is irritate the reader by making him/her look up things. Make it UNDERSTANDABLE!
- j. Allow PLENTY of time. Everything will take 3 to 5 times longer than you think.

Sample Approval Page: Student must prepare this page prior to presentation and give it to committee at the presentation. Must be turned into Graduate Advisor.

(Allow 2" top margin)

THE TITLE IS IN ALL CAPS, NO MORE THAN 48 CHARACTERS SPACES
TO A LINE, CENTERED BETWEEN MARGINS, DOUBLE SPACED
ARRANGED IN AN INVERTED PYRAMID SHAPE

Chemistry 7334 – Proposal Methodology

Student Name

Date of presentation (*italics*)

Result:

_____ PASS

_____ CONDITIONAL PASS (conditions for Pass must be precisely specified
below or on attached pages and a date for completion given)

_____ FAIL COMMENTS:

Approved by: (Allow adequate space for signatures)

Single space name & title below line

List Advisor first, others alphabetical order

List in alphabetical order

List alphabetical order

Fourth line only if committee member outside of Chemistry
Department is included

CHEM 7111 and 7112

Teaching Practicum

All students are required to teach at least two semesters with between 10 and 25 hours per week with duties that include laboratory preparation; active interaction with students during laboratory sessions; grading of exams, homework and lab reports; proctoring exams in lecture sections; preparing demonstrations for lecture sections; etc. Teaching assignments are made at the beginning of each semester and teaching assistants are expected to attend weekly TA meetings in addition to the activities listed above. While more specific directions will be provided by the TA supervisor to whom each student is assigned, some general guidelines are discussed below. The main objective is to improve the graduate student's communication and evaluation skills. **The performance of each teaching assistant is reviewed each semester.**

1. Learn the safety rules for your assigned duties. Always wear safety glasses.
2. Wear the correct personal protection.
 - Wear safety glasses AT ALL TIMES when in the laboratory.
 - Wear lab coats AT ALL TIMES when in the laboratory
 - No shorts or miniskirts.
 - No open toed sandals or flip flops.
 - No loose clothing.
 - Tie back long hair.
 - No food or drinks.
3. Location of safety equipment.
Know the location of the safety showers, eye washes, and fire extinguishers and how to use each of them.
4. Use proper technique and listen to instructions carefully.
You are an example to the students, and they will copy whatever you are doing. At no time should you take a "short cut" at the expense of doing something safely. Know how to use each piece of equipment or technique safely and be able to demonstrate it to the students. (Bunsen burner, gravity filtration, suction filtration, titration, etc.) Know how and where waste should be disposed. A short summary of the experiment, its calculations, and common questions or errors will be given preceding the lab.
5. You are expected to attend weekly TA meetings.
6. At all times you should act professionally. A courteous, respectful, and cheerful attitude is most helpful.
 - You can be friendly and joke around with students without acting inappropriately.
 - Treat the students fairly, and do not play favorites.
 - Do not single out or embarrass a student if they have made an error, but be quick to speak to them if they are behaving in an unsafe manner.
 - Try to answer the students' questions as best as possible (but don't give away answers), and do not tell a student their question was dumb. Be as patient as possible with them.
 - A word to the wise: be very careful what you put up on Facebook and what you have written on your "walls". Remember that potential employers can see this, too.
7. Grading student work
 - Grade fairly. Do not play favorites. Try not to look at names on the papers.
 - Read the student's answer thoroughly. They may have the right answer, but it may not be worded exactly as the key.
 - Take off the same amount of points for similar errors. Most keys will have point counts on them. Take time to look back at papers you graded earlier to check that you are consistent.

- It is helpful to grade all of the same type of quiz (and laboratory report) at one time for consistency.
 - The instructor will check grading on two to three sets. Incorrect grading will result in a lower course grade in Chem 7111 and 7112.
8. Your course grade for Chem 7111 and 7112 will be based on the following:
- Interaction with students.
You will be evaluated by the instructor on your interaction with students and overall behavior in the course (communication skills, patience with students, demeanor). The undergraduate students in your class will also complete an evaluation for you at the end of the course (see below.)
 - Preparation for lab.
You will be expected to be prepared for each lab. You should read the lab thoroughly and be able to clearly explain each procedure to the students. In addition, you should do each homework problem (factor label method for all calculations) and be able to explain this to the students.
 - Safety in the lab.
You will be expected to observe and uphold all safety rules.
 - Grading of student papers.
You will be expected to grade some homework and quizzes. The instructor will check grading on two to three sets. Incorrect grading will result in a lower course grade.
 - TA paper.
You will be expected to write a paper on your TA experience (details will be provided each semester). The fall term paper is due on or before the first Monday in December.
 - **Professionalism and overall seriousness of approach to this assignment.**
 - Other criteria
If you are assisting on the laboratory preps, your accuracy making solutions, cleaning glassware, and setting up will be evaluated.