Chem 402/5020
Physical Chemistry II

SP2025

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1 Course Description

Intro to the properties and kinetic theory of gases, chemical thermodynamics, and statistical mechanics.

1.1 Prerequisites

Required course for all Chemistry majors. Prereqs.: Chem 111A-112A (or Chem 105-106 with permission of instructor), Chem 401, and Math 233; or permission of instructor. Prior completion of Physics 191-192 (or Physics 193-194) is strongly encouraged, but prior completion of Physics 191/193 and concurrent enrollment in Physics 192/194 will be accepted. Graduate students interested in this course should enroll in the graduate level course, Chem 5020.

1.2 Learning Goals

By the end of this course, students should be able to:

1. **Recall and Explain Core Thermodynamic Principles**
    - Recall and define key thermodynamic variables (e.g., temperature, pressure, volume) and fundamental laws (First, Second, Third), describing how each underpins chemical phenomena.
    - Explain the physical significance of concepts such as internal energy, enthalpy, entropy, Helmholtz and Gibbs free energies, and their roles in predicting system behavior.
2. **Apply Equations of State to Real Systems**
    - Apply the ideal gas law to solve quantitative problems under idealized conditions.
    - Use real gas equations (van der Waals, Redlich-Kwong, Virial, etc.) to predict deviations from ideality and evaluate when these corrections are necessary.

- Interpret compressibility factors and virial coefficients to characterize non-ideal behavior in gases.

3. **Analyze Statistical Foundations**
    - Analyze the assumptions and derivations of the kinetic theory of gases to connect microscopic motion to observable macroscopic properties (e.g., pressure and temperature).
    - Interpret Maxwell–Boltzmann distributions in terms of energy, velocity distributions, and temperature dependence.
    - Compare how statistical mechanics (e.g., partition functions and Boltzmann factors) underlies the thermodynamic equations of state.
4. **Derive and Evaluate Thermodynamic Relationships**
    - Derive important thermodynamic identities and Maxwell relations from the fundamental potentials.
    - Evaluate how partial derivatives relate to measurable quantities such as heat capacity, compressibility, and expansion coefficients.
5. **Predict and Interpret Phase Behavior**
    - Interpret single- and multi-component phase diagrams (e.g., pressure-temperature diagrams) to identify critical points, triple points, and phase boundaries.
    - Compare phase transitions (e.g., melting and boiling) and quantify changes in enthalpy and entropy at those boundaries.
    - Apply the Clapeyron or Clausius–Clapeyron equations to predict phase transition lines and interpret how temperature and pressure shifts affect equilibrium.
6. **Assess Chemical Equilibria Using Thermodynamics & Statistical Mechanics**
    - Calculate reaction equilibria from Gibbs energies and relate changes in temperature or pressure to shifts in equilibrium using the van't Hoff equation.
    - Compare reaction quotients to equilibrium constants and predict the direction of spontaneous change.
    - Relate microscopic partition functions to macroscopic equilibrium constants, describing how molecular-level interactions define bulk reaction behavior.

7. **Solve Quantitative and Conceptual Problems in Thermodynamics**
    - Solve numerical problems involving heat capacity, work, heat, and energy changes under isothermal, adiabatic, and other processes, justifying each step with thermodynamic laws.
    - Construct and interpret pressure-volume diagrams or other thermodynamic plots to visualize expansions, compressions, and cycles (e.g., Carnot cycle).
    - Employ approximation techniques (e.g., Stirling's approximation) and probability distributions in statistical mechanics to tackle complex problems.
8. **Evaluate Real-World Applications & Integrate Knowledge**
    - Evaluate how thermodynamic principles inform processes like the Haber–Bosch synthesis, phase separations in environmental contexts, or biochemical equilibria.
    - Integrate thermodynamics with statistical mechanics in discussing modern technology (e.g., sustainable energy solutions, electrochemical cells) and research directions.

1.3 Literacies for Life and Career

1. **Applied Problem Solving**: Throughout this course, students use theoretical models and computational frameworks to represent, evaluate, and solve complex chemical problems. Whether deriving equations of state from microscopic principles or computing equilibrium constants from partition functions, they learn to identify assumptions, choose appropriate analytical tools, and validate their results against experimental or literature data.
2. **Data Analysis**: The course emphasizes the interpretation of experimental and simulated data, from understanding temperature-pressure-volume relationships in gases to extracting thermodynamic properties (e.g., entropies, enthalpies) from statistical and thermodynamic models. Students gain proficiency in utilizing quantitative methods, exploring uncertainties, and discerning patterns in both theoretical predictions and empirical measurements.
3. **Systematic Inquiry**: By approaching chemical questions from first principles and employing structured methodologies—such as defining ensembles, writing down rigorous thermodynamic relationships, and systematically testing hypotheses—students practice inquiry-driven learning. They refine their ability to design and interpret experiments or simulations, connect theoretical models with observed phenomena, and contribute to a deeper understanding of physical chemical systems.

2 Texts, Materials, and Supplies

Physical Chemistry: A Molecular Approach, Donald A. McQuarrie and John D. Simon

[This textbook was used for the first semester Chem 401/5010 course.]

3 Grading

3.1 Final Grade Composition

- **7 Problem Sets (30 points each)**
- **2 Midterm Exams (100 points each)**
- **1 Final Exam (150 points)**

Table 1 shows the *maximum* grade boundaries.

%	Grade
[90, 100]	A
[85, 90)	A-
[80, 85)	B+
[70, 80)	B
[65, 70)	B-
[60, 65)	C+
[50, 60)	C
[45, 50)	C-
[40, 45)	D+
[30, 40)	D
[25, 30)	D-
[0, 25)	F

Table 1: *Maximum* Grade Boundaries

3.2 Regrading Requests

Regrade requests must be submitted in writing within one week of receiving the graded work. The entire assessment will be re-evaluated, which may lead to an adjustment in the final score.

3.3 Missed Exams

Students must notify the instructor as soon as possible if they anticipate missing an exam. Make-up exams will only be granted with valid documentation.

4 Assignments and Homework

The general expectation is that students will spend at least six to nine hours outside class studying and doing homework and projects.

4.1 Homework Assignments

Each homework assignment consists of problems that challenge you to derive relationships between statistical mechanical and thermodynamic variables and functions, apply these or given relationships for practical calculations, and use software (e.g., Microsoft Excel, WolframAlpha, and desmos) and standard reference databases (e.g., National Institute of Standards and Technology). These assignments are crafted to enhance your analytical, mathematical, and practical skills, deepen your understanding of course concepts, and apply them to solve real-world chemical problems.

4.2 Graduate Student Requirements

- **Context**: Reading *Einstein's Fridge* by Paul Sen (ISBN13: 9781501181313) and discussing the historical context of statistical thermochemistry on Canvas.
- **Advanced Assignments**: More demanding, integrating computational, numerical, and theoretical methods and data analysis to draw conclusions from complex datasets and developing Python code for advanced problems and simulations.

4.3 Late Assignments

Late assignments will incur a 5% penalty per day up to a maximum of three days. Extensions may be granted for valid reasons, but requests must be submitted before the original due date.

5 Attendance, Participation, and Classroom Climate

While class participation and attendance do not factor into course grades, attendance is mandatory as these are vital components of this course.

5.1 Weekly Office Hours

I, along with the AIs, will host weekly office hours **on a TBD day and time in Jolley 431**. These opportunities allow you to seek additional help, discuss course material in depth, or get feedback on your assignments.

Your regular attendance and active participation in weekly office hours will enrich your learning experience and foster a collaborative and engaging classroom culture. Engaging consistently in this component of the course will significantly enhance your understanding and proficiency in statistical thermochemistry.

6 Feedback Mechanisms

Students are encouraged to provide feedback through weekly minute papers and a midterm course evaluation. These tools allow for anonymous input on course content, pacing, and teaching effectiveness. I will use this feedback to make timely adjustments and ensure the course meets student needs. Feedback on assignments will be provided promptly with clear explanations, and detailed solutions with point breakdowns will be shared three days after assignments are due.

7 Course Calendar

Table 2: Tentative Course Calendar

Week	Date	Module	Topic
1	1/13/25	1	Equations of State
2	1/20/25		Martin Luther King, Jr. holiday (no classes)
3	1/27/25	2	Statistical Mechanics

Continued on next page

Table 2 – *Continued from previous page*

Week	Date	Lecture	Topic
5	2/14/25	3	First Law & Enthalpy
5			**First Exam (6:00–9:00 PM, Louderman 458)**
7	2/26/25	4	Second Law & Entropy
9	3/10/25		Spring Break (no classes)
9	3/12/25		Spring Break (no classes)
9	3/14/25		Spring Break (no classes)
10	3/17/25	5	Third Law & Free Energy
10	3/20/25		**Second Exam (6:00–9:00 PM, Louderman 458)**
11	3/24/25	6	Phase Equilibria
12	4/2/25	7	Chemical Equilibria
14	4/14/25		Passover (TBD)
14	4/16/25	8	Special Topics
	5/5/25		**Final Exam (10:30 AM–12:30 PM)**

8 University-Wide Policies & Guidelines

8.1 COVID-19 Health and Safety Protocols

Students experiencing symptoms consistent with COVID-19 or concerned about a possible exposure should contact Habif Health and Wellness Center (314 935-6666) to arrange for testing

as indicated. If a student tests positive for Covid-19, they will receive a letter with instructions about any necessary isolation that they can share with their instructors. **Update: 9/1/23. Illness activity at the start of the semester is high, and students may not have documentation of their COVID status; instructors should NOT request students provide them with results of PCR tests in order to receive an excused absence. During this time, please extend grace to students who indicate a need to isolate and allow their absence so that we may reduce the likelihood of illnesses being transmitted in our classrooms.** Any accommodation needs for COVID-related absence not covered in an instructor's standard course policies should be discussed between the student and instructor.

While on campus, it is imperative that students follow all public health guidelines established to reduce the risk of COVID-19 transmission within our community. The full set of University protocols can be found on the Health and Safety webpage. This includes:

Masking;

Masking remains a valuable tool in the mitigation of COVID-19, particularly in light of new and emerging variants. Students and instructors are encouraged to treat requests to mask with care and consideration, keeping in mind that some individuals may be at a higher risk, caring for others at a higher risk, or feeling less comfortable in a mask-optional environment. Based on monitoring of regional and campus conditions, a mask requirement may be implemented as needed.

Students with disabilities for whom masked instructors or classmates create a communication barrier are encouraged to contact Disability Resources (www.disability.wustl.edu) or talk to their instructor for assistance in determining reasonable adjustments. Adjustments may involve amplification devices, captioning, or clear masks but will not allow for the disregard of mask policies should a requirement be in place.

8.2 Reporting Sexual Assault and Harassment

If a student discusses or discloses an instance of sexual assault, sex discrimination, sexual harassment, dating violence, domestic violence or stalking, or if a faculty member otherwise observes or becomes aware of such an allegation, the faculty member will keep the information as private as possible, but as a faculty member of Washington University, they are required to immediately report it to the Department Chair or Dean or directly to Ms. Cynthia Copeland, the University's

Associate Title IX Coordinator, at (314) 935-3411, cmcopeland@wustl.edu. They will also offer available resources, including confidential support resources through the Relationship and Sexual Violence Prevention (RSVP) at 314-935-3445. Additionally, you can report incidents or complaints to the Office of Student Conduct and Community Standards or by contacting WUPD at (314) 935-5555 or your local law enforcement agency. See: Gender Equity and Title IX Compliance Office

8.3 Disability Resources (DR)

WashU supports the right of all enrolled students to an equitable educational opportunity, and strives to create an inclusive learning environment. In the event the physical or online environment results in barriers to the inclusion of a student due to a disability, they should notify the instructor as soon as possible.

Disabled students requiring adjustments to equitably complete expectations in this course should contact WashU's Disability Resources (DR), and engage in a process for determining and communicating reasonable accommodations. Because accommodations are not applied retroactively, DR recommends initiating requests prior to, or at the beginning of, the academic term to avoid delays in accessing accommodations once classes begin. Once established, responsibility for disability-related accommodations and access is shared by Disability Resources, faculty, and the student.

Disability Resources: www.disability.wustl.edu; 314-935-5970

8.4 Statement on Military Service Leave

Washington University recognizes that students serving in the U.S. Armed Forces and their family members may encounter situations where military service forces them to withdraw from a course of study, sometimes with little notice. Students may contact the Office of Military and Veteran Services at (314) 935-2609 or veterans@wustl.edu and their academic dean for guidance and assistance. See: https://veterans.wustl.edu/policies/policy-for-military-students/.

8.5 Preferred Name and Personal Pronouns

Washington University in St. Louis recognizes that many students prefer to use names other than their legal ones to identify themselves. In addition, in order to affirm each person's gender identity and lived experiences, it is important that we ask and check in with others about

pronouns. This simple effort can make a profound difference in a person's experience of safety, respect, and support. See: Pronouns Information and Preferred Name.

8.6 Emergency Preparedness

Before an emergency, familiarize yourself with the building(s) that you frequent. Know the layout, including exit locations, stairwells and the Emergency Assembly Point (EAP). Review the "Quick Guide for Emergencies" that is found near the door in many classrooms and main lobby areas of buildings for specific emergency information and instructions. For additional Information and EAP maps, visit https://emergency.wustl.edu/. To ensure that you receive emergency notifications, make sure your information and cell phone number is updated in SIS, and/or download the WashU Safe app and enable notifications.

To report an emergency:

Danforth Campus: (314) 935-5555

School of Medicine Campus: (314) 362-4357

North/West/South and Off Campus: 911 then (314) 935-5555

8.7 Academic Integrity

Effective learning, teaching and research all depend upon the ability of members of the academic community to trust one another and to trust the integrity of work that is submitted for academic credit or conducted in the wider arena of scholarly research. Such an atmosphere of mutual trust fosters the free exchange of ideas and enables all members of the community to achieve their highest potential.

In all academic work, the ideas and contributions of others (including generative artificial intelligence) must be appropriately acknowledged and work that is presented as original must be, in fact, original. Faculty, students and administrative staff all share the responsibility of ensuring the honesty and fairness of the intellectual environment at Washington University in St. Louis.

For additional details on the university-wide Undergraduate Academic Integrity policy, please see: https://wustl.edu/about/compliance-policies/academic-policies/undergraduate-student-academic-

integrity-policy/

For information specific to the College of Arts & Sciences please refer to the A&S Academic Integrity webpage.

Turnitin

In taking this course, students may be expected to submit papers and assignments through Turnitin for detection of potential plagiarism and other academic integrity concerns. If students do not have an account with Turnitin and/or do not utilize Turnitin when submitting their papers and assignments, the instructor may upload your paper or assignment to Turnitin for processing and review.

9 Resources for Students

9.1 Confidential Resources for Instances of Sexual Assault, Sex Discrimination, Sexual Harassment, Dating Violence, Domestic Violence, or Stalking

The University is committed to offering reasonable academic accommodations (e.g. a no-contact order, course changes) to students who are victims of relationship or sexual violence, regardless of whether they seek a formal investigation or criminal charges. If a student needs to explore options for medical care, other services, or reporting, or would like to receive individual counseling services, there are free, confidential support resources and professional counseling services available through the Relationship and Sexual Violence Prevention (RSVP) Center. If you need to request such accommodations, please contact RSVP to schedule an appointment with a confidential and licensed counselor. Although information shared with counselors is confidential, requests for accommodations will be coordinated with the appropriate University administrators and faculty. The RSVP Center is located in Seigle Hall, Suite 435, and can be reached at rsvpcenter@wustl.edu or (314) 935-3445. For after-hours emergency response services, call the Sexual Assault and Rape Anonymous Helpline (SARAH) at (314) 935-8080 or call 314-935-6666 or (314) 935-5555 and ask to speak with an RSVP Counselor on call. See: RSVP Center.

9.2 Bias Reporting and Support System (BRSS)

The University has a process through which students, faculty, staff, and community members who have experienced or witnessed incidents of bias, prejudice, or discrimination against a student can report their experiences to the University's Bias Report and Support System (BRSS) team.

9.3 Counseling and Psychological Services

Counseling and Psychological Services' professional staff members work with students to resolve personal and interpersonal difficulties, many of which can affect a student's academic experience. These include conflicts with or worry about friends or family, concerns about eating or drinking patterns, and feelings of anxiety, depression, and thoughts of suicide. Individual, Conjoint, and Group therapy are all provided in addition to referrals for off-campus support. Information can be found on the Mental Health Services webpage.

The Division of Student Affairs also offers a telehealth program to students called TimelyCare. While students are encouraged to visit Counseling and Psychological Services during business hours, this additional service also provides after-hours access to medical care and 24/7 access to mental telehealth care across the United States, with no cost at the time of the visit. 12 counseling visits are provided at no charge as well as a limited number of psychiatry appointments. Students who pay the Health and Wellness fee are eligible for this service.

Additionally, see the mental health services offered through the RSVP Center listed above.

9.4 WashU Cares

WashU Cares specializes providing referrals and resources, both on, and off campus for mental health, medical health, financial and academic resources by using supportive case management. WashU Cares also receives reports on students who may need help connecting to resources or whom a campus partner is concerned about. If you are concerned about a student or yourself, you can file a report here: https://washucares.wustl.edu/.

9.5 The Writing Center

The Writing Center offers free writing support to all Washington University undergraduate and graduate students. Staff members will work with students on any kind of writing project, including essays, writing assignments, personal statements, theses, and dissertations. They can help at any stage of the process, including brainstorming, developing and clarifying an argument,

organizing evidence, or improving style. Instead of simply editing or proofreading papers, the tutors will ask questions and have a conversation with the writer about their ideas and reasoning, allowing for a higher order revision of the work. They will also spend some time looking at sentence level patterns to teach students to edit their own work.

The Center is located in Mallinckrodt and open Sunday through Thursday from 11:00 am to 9:00 pm and Friday from 11:00 am to 5:00 pm. Students are seen primarily by appointment, with walk-ins accepted as the schedule allows. They also have dedicated walk-in hours for undergraduates on Tuesday and Wednesday afternoons. Both in-person and online appointments are available. To make an appointment, go to writingcenter.wustl.edu. Email: writing@wustl.edu.

9.6 The Learning Center

The Learning Center provides peer-led support programs, including course-specific mentoring and academic skills coaching (study and test-taking strategies, time management, etc.), that enhance undergraduate students' academic progress. Contact them at learningcenter@wustl.edu or visit ctl.wustl.edu/learningcenter to find out what support they may offer for your classes.

9.7 Center for Diversity and Inclusion (CDI)

The Center for Diversity and Inclusion (CDI) supports and advocates for undergraduate, graduate, and professional school students from underrepresented and/or marginalized populations, collaborates with campus and community partners, and promotes dialogue and social change to cultivate and foster a supportive campus climate for students of all backgrounds, cultures, and identities. Additional Diversity and Inclusion information can be found at https://diversityinclusion.wustl.edu/.

9.8 Gephardt Institute

Students play an essential role in a vibrant and functioning democracy! State and local elections take place throughout the year and have a direct impact on our communities. You can register to vote, request an absentee ballot, confirm your polling location, and get Election Day reminders at http://wustl.turbovote.org for any of the 50 states and Washington D.C. WashU students are considered Missouri residents, and eligible student voters can register to vote in the state of Missouri or their home state.

If you are ineligible to vote, you can participate by encouraging your friends to register and vote, engaging your peers in local issues, and taking part in other civic and community engagement ac-

tivities. For more resources on voting and other civic and community engagement opportunities, please visit http://washuvotes.wustl.edu and http://gephardtinstitute.wustl.edu.

9.9 University Libraries

University Libraries include seven unique locations across the Danforth Campus, but they are much more than just beautiful, quiet spaces for studying and group work. The Libraries include librarians for every discipline on campus, with the expertise to work with you to develop research ideas and find the best resources to meet your needs; or you are welcome to explore our research guides, tailored for each subject and available online. The Libraries hold five million items in the collection—print books, journals, electronic resources, databases, and millions more accessible through interlibrary loan—and you can find it all at the search on our home page. Additional resources for students include special collections, data services, citation help, digital publishing, and more. Visit the Libraries website for more details about these and other ways that the Libraries are here to support your academic success. Electronic resources listed on the Libraries' website and catalog are restricted to current students, staff, and faculty for the purposes of research, teaching, and private study. For more information, please visit https://libguides.wustl.edu/RERU

Chemistry Subject Librarian: Rhiannon Iha, (314) 935-4818, rkiha@wustl.edu

10 Additional Considerations

10.1 Religious Holidays & Class Absence Policies

As home to students, faculty, and staff of all the world's major religions and as a non-sectarian institution, Washington University in St. Louis values the rich diversity of spiritual expression and practice found on campus. It is therefore the policy of the university that students who miss class, assignments, or exams to observe a religious holiday should be accommodated as follows:

(i) absences should be counted as excused in any course in which attendance is a measure of academic performance;

(ii) reasonable extensions of time should be given, without academic penalty, for missed assignments;

(iii) exams should be reasonably rescheduled without academic penalty.

To ensure that accommodations may be made, students who plan to miss class for a religious holiday must inform their instructors in writing before the end of the third week of class, or as

soon as possible if the holiday occurs during the first three weeks of the semester. Absence for religious reasons does not lessen students' responsibility for course work or material covered during their absence. It is incumbent on the student who misses a class to catch up on any material discussed and assignments given during that class period. If you believe you have not received a reasonable accommodation despite engaging with your instructor on the topic, please follow the course grievance process outlined by your school.

Every effort will be made to avoid scheduling exams on religious holidays, particularly those with work restrictions as noted on the holiday calendar. Where it is not possible to establish a teaching schedule that avoids conflict with the observance of religious holidays, the instructor will make up any missed class in the method most appropriate to student learning in their course; e.g., rescheduling for an alternate time, providing asynchronous material, or engaging a guest lecturer. Appropriate advance notice will be provided to students.

The complete Religious Holiday Class Absence Policy can be found here. The Office of Religious, Spiritual and Ethical Life maintains a calendar of many religious holidays observed by the WashU community.