1. Course Information

Course Code & Name: Chem350, Quantum Chemistry

Semester & Year: Spring 2017

Time: Wednesdays 08:40-10:30, Fidays 10:40-12:30

2. Instructor Information

Section 1 (K-15)

Name: İlker Özkan

Office Address: 0-222 Chemistry

Office Hours: No fixed office hours. Take appointment (through e-mail) before coming to my office

e-mail: ilker@metu.edu.tr

3. Course Description

Particles and waves, principles of quantum mechanics, stationary states. Electronic structure of atoms and molecules. The chemical bond. Approximate methods. Vibrational, rotational and electronic transitions. Spectroscopy.

4. Course Materials & Resources

Textbook:

Lecture notes prepared by Prof. İlker Özkan will be used throughout this course. Lecture notes for each topic/chapter will be provided to you via ODTÜClass in pdf format.

Refrence textbooks:

Physical chemistry Keith J. Laidler, John H. Meiser, Bryan C. Sanctuary. Laidler, Keith James, Boston: Houghton Mifflin, c2003. Call no: QD453.3 .L35 2003 (will be referred to as **LKJ**)

Physical chemistry Atkins, P. W., de Paula J., Oxford University Press, 2006.
Call no: QD453.2 .A88 2006 (8th edition) (will be referred to as **A**)
Online Resource Center: http://www.oup.com/uk/orc/bin/9780198700722/

Physical chemistry : a molecular approach McQuarrie, Donald A., Sausalito, Calif. : University Science Books, c1997. Call no: QD453.2 .C87 1997 (will be referred to as **M**)

Molecular quantum mechanics Atkins, P. W., Oxford University Press, 2005.
Call no: QD462 .A85 2005, Online Resource Center: http://www.oup.com/uk/orc/bin/9780199274987/

Quantum chemistry Levine, Ira N., 1937- Upper Saddle River, N.J. : Prentice Hall, c2000.
Call no: QD462 .L48 2009 (6th edition) (will be referred to as **L**)

Fundamentals of physics Halliday, D., Resnick R., Walker J.,John Wiley Sons Inc., 2008.
Call no: QC21.3 .H35 2005 (7th edition) (8th edition will be referred to as **H**)

The chemistry maths book Steiner, E., Oxford ; New York : Oxford University Press, 2008.
Call no: QA37.2 .S7985 (2nd edition) (will be referred to as **S**)
Electronic version can be accessed at:
http://library.metu.edu.tr/search~S4?/asteiner/asteiner/1%2C90%2C178%2CZ/l856&FF=asteiner+erich+1937&3%2C%2C4%2C1%2C0

Other resources:

Mathcad: This is a powerful and easy to use/learn math software. Since it is based on a visual input format that uses standard mathematical notation (rather than text input that many other math software,

like *Mathematica*, use) it is very easy to learn how to use it. ***Mathcad* is installed in all the computers in the chemistry computer lab**.

5. Contents

Section numbers corresponding to each topic, from the references given above, are indicated in parantheses, next to topic titles.

5.3.3 Vibrational wavefunctions and Quantum Mechanical tunneling
5.3.4 Selection rules in vibrational transitions
5.4 Vibration-Rotation Spectra of Diatomic Molecules (A 13.9, 13.10, 13.12, LKJ p.673-677)
Appendix. Kinetic energy in the vibrational motion of a diatomic molecule
Suggested problems:
From LKJ: Problems: 13.18, 13.21, 13.23, 13.25,
From A: Exercies: 9.13a, 9.15a,; Problems: 9.2, 9.12, 9.19,
From L: Problems: 4.4, 4.7, 4.10, 4.19, 4.23, 4.25

6 Hydrogen Atom
6.1 Coulomb interaction energy among charged particles in an atom or a molecule (L 13.3)
6.1.1 Coulomb interaction energy for an atom in atomic units
6.1.2 Coulomb interaction energy for a molecule in atomic units
6.1.3 Kinetic energy operator for an electron in atomic units
6.2 Allowed energy levels of the electron in H-atom (L 6.5-6, S 14.6, A 10.1-2, LKJ 11.7-8)
6.2.1 The radial functions R(r)
6.2.2 Dependence of Atomic Orbitals on the angular variables
6.3 Energy levels and radial functions in hydrogenlike atoms (L 6.7, A 10.1-2, LKJ 11.7-8)
Suggested problems:
From LKJ: Problems: 11.40, 11.42, 11.43, 11.44, 11.48,
From A: Exercies: 10.1a, 10.2a, 10.4a, 10.5a, 10.6a, 10.8a; Problems: 10.3, 10.11, 10.15, 10.17, 10.25
From L: Problems: 6.1, 6.15, 6.26, 6.28, 6.32, 6.33, 6.34, 6.35, 6.37, 6.41

7 Many Electron atoms
7.1 Electronic states of helium atom
7.2 The Variation Method (LKJ 564-565, L 8.1)
7.3 Total Orbital and Spin Angular Momenta in an Atom (L 11.4)
7.3.1 The total orbital angular momentum of electrons in an atom (L 11.4)
7.3.2 The total spin angular momentum of N electrons (L 10.1)
7.3.3 The Pauli Exclusion Principle (A 10.4.b, L 10.3, LKJ p. 558-560)
7.4 Designing trial variation functions for the helium atom
7.4.1 Two-electron spin functions (L 10.4, p. 333-335,A 10.7)
7.4.2 Two-electron functions of spatial variables
7.4.3 Ground state of He atom
7.4.4 Excited electronic states of He atom
7.5 The term with the lowest energy: Hund's Rule (L p. 332-333)
7.6 Atomic term symbols for N>2 electrons
7.7 The total angular momentum J and atomic energy levels (L 11.6, A 10.8)
7.8 Selection rules for transitions between atomic energy levels in absorption or emission of light.
Suggested problems:
From A: Exercies: 10.9a, 10.10a, 10.12a, 10.14a, 10.15a, 10.16a, 10.17a, 10.18a, 10.19a
From L: Problems: 11.6, 11.11, 11.13, 11.19, 11.20, 11.21, 11.22, 11.23, 11.26, 11.29

8 Electronic States of Molecules
8.1 The Born-Oppenheimer approximation (L 13.1, LKJ p. 580
8.1.1 The electronic Schrödinger equation
8.1.2 The Schrödinger equation for the nuclei
8.2 Electronic states of the hydrogen molecule (L 13.7, 13.8, A 11.3, LKJ p. 590-593)
8.2.1 The orbital approximation in molecules: Molecular Orbitals
8.2.2 Molecular Orbitals as Linear Combination of Atomic Orbitals (LCAO)
8.2.3 Low-lying electronic states of H_2
8.3 Homonuclear diatomic molecules of Period 2 atoms (L 13.7, 13.8, A 11.4, LKJ p. 622-626)
8.3.1 Term symbols of homonuclear diatomic molecules
Suggested problems:
From A: Exercies: 11.1a, 11.1b, 11.3a, 11.3b, 11.5b,
From L: 13.1, 13.2, 13.2, 13.4, 13.24, 13.25, 13.26, 13.27

9 Hückel π-electron MO theory for conjugated hydrocarbons

9.1 Hückel Molecular Orbitals
9.2 Writing Hückel equations for the LCAO coefficients in the general case

6. Exams and Grading Policy

Your performance in this course will be assessed by two midterms and a final examination, with weights shown below.

Midterm 1: on Sunday, March 26, 2017 at 13:00	30%
Midterm 2: on Sunday, April 30, 2017 at 13:00	30%
Final Examination: to be determined	40%

Each exam grade will be announced out of a maximum of 100 points.

Not everyone will be permitted to take the final exam: There are 54 class hours for Chem350 during the 2017 Spring semester. Your attendance to the classes will be carefully monitored. You must attend to at least 32 lecture hours out of a maximum of 54. If you fail to satisy this condition, a) You will not be allowed to take the final examination; b) your letter grade will be assigned as "NA" in your record.

Please note that in counting the attendance no excuses (including medical) will be taken into consideration.

- While assigning the letter grades, average grade of the class and the spread of the grades will be taken into account. This doesn't necessarily mean that the average score will get CC but rather should be considered as a "modified catalog". **Finally regardless of the class average, a total score of less than 45 will fail. This does not necessarily mean that any score above 45 will pass (passing score may depend on the class average). If you try to negotiate about your grade during the grading period at the end of the term, official grading and attendance rules (see METU Academic Catalog, Article 10) will be applied.**
- Make up exam will be given, after the finals period, **only** to those students who have a **valid, officially documented excuse** (see METU Academic Catalog, Article 9). Unfortunately each term there exist some who miss the passing grade by just 1 or 2 points. At the end of this term, if you happen to be one of those, please **don't** come to my office just before the grades are submitted and ask for an extra/make up exam to raise your grade.
- All announcements (grades, assignments,...) will be posted on "ODTUCLASS" website (and when possible via e-mail), and you are expected to check ODTUCLASS and METU e-mail accounts regularly (weekly).

7. University Policies

It is very important that you know and understand the university regulations regarding academic integrity, since you are expected to and should act according to these rules throughout your university life. Below I quoted the abovementioned academic integrity code.

Code of Integrity ****
All students are expected to have academic integrity principle in all academic works. That is, a student must submit work only the student's own. Students shall comply with academic integrity codes and shall avoid situations likely to violate this code since academic dishonesty diminishes credit to the academic community.

Academic Dishonesty
Academic dishonesty is defined as any activity, which tends to undermine the academic integrity of the university. Academic integrity is one of the major factors that determines the image and dignity of the university. So not only

academic people are responsible to maintain the duration of academic integrity, all members of the university including students should obey the rules and regulations of the university.

Academic Misconducts
Behaviour considered as misconduct or violation in academic terms are defined so:

a. Cheating

Cheating means giving or receiving any unauthorized aid in any academic exercise. It includes but is not limited to the following actions:

- *Copying from someone else's test or examination paper*
- *Using external assistance like the use of tutors, books, lecture notes and calculator in any in-class or take-home examination although it is prohibited*
- *Possessing, buying, selling, removing, receiving or using a copy or copies of any materials to be used as an instrument of academic evaluation*
- *Using another person as a substitute in an academic evaluation*
- *Working with other persons on a particular project although the instructor has required indivudial work*
- *Copying a report or homework assignment prepared by someone else or using records or laboratory results obtained by someone else as it is your work*
- *Attempting to influence or change any academic evaluation by unfair means which includes altering exam results or grades or changing anything on exam papers hiddenly while they are shown by the instructor for control and objections*

b. Plagiarism

Plagiarism means using a part or whole of a written material without proper acknowledgement of source. A student should pay attention to the originality of any material he or she uses for such situations:

- *Whenever he or she quotes another person's actual words,*
- *Paraphrases another person's words,*
- *Uses another person's idea, opinion or theory,*
- *Whenever he or she uses internet sources, borrows facts, statistics or any information which is not common knowledge.*
- *As a whole, theses, essays, term papers, and other academic project requirements must be the original work of the student who is submitting them. And while using other materials, the source should be properly and clearly defined by references.* For useful information regarding plagiarism check http://www.fbe.metu.edu.tr/Intihal/intihal.htm

3. Fabrication

Fabrication is defined as intentionally misrepresentation of any academic information or citation in order to deceive. A student must not falsify or invent any information or data in an academic exercise including, but not limited to, records or reports, laboratory results, and citations to the sources of information.

4. Interference
Interference is defined as trying to get advantage in any academic evaluation by unfair ways. This includes but is not limited to the following:

- *A student should not steal, change or destroy another student's work. This includes theft, defacement, harming or collecting all sources so as to prevent others to reach the information they contain.*
- *A student should not give or offer bribe, promise favors, make threats to any academic staff to change or affect any grade or result of any academic evaluation.*

5. Facilitating Academic Dishonesty

This means aiding or abetting others to cheat, to plagiarise or to commit any academic dishonesty. A student must not intentionally or knowingly help or attempt to help another student to commit an act of academic misconduct. It includes but is not limited to the following:

- *Giving unauthorized assistance to another or others during an academic evaluation like allowing students to copy from each other or lecture books or notes.*
- *Substituting for another student in an academic evaluation.*
- *Permitting one's academic work to be represented as the work of another.*

- *Providing any information about any academic evaluation before it takes place to a student such that that person gains an advantage for academic evaluation.*

6. Responsibility to Report Academic Dishonesty

Universities are academic entities which are devoted to innovate and transmit new knowledge for the scientific, technological, economic, cultural and social improvement of the society through scholarly research and related community services. The responsibility is to maintain an environment in which it members should behave in a good manner.

Academic Dishonesty is a serious threat to the dignity of the university. It decreases the quality of education and causes loss of confidence in terms of university premises. That's why it is the responsibility of all students to report any witnessed academic dishonesty. If one does not comply with university rules and regulations and academic misconducts stated above and if another one sees or realises this and does not report it to any academic unit, he or she will be a part of the violation committed against university's integrity.

* The parts in italic are adapted from the Instruction Technology Services Office website with minor modifications.

** The parts in italic are quoted from the METU Student Code of Conduct published by the METU Ethics Club.