Chemistry 611
Physical Inorganic Chemistry
Course Syllabus
Spring 2018
(first draft)

1. General Information

Instructor: Andy Pacheco
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Recommended Text: *Shriver and Atkins' Inorganic Chemistry, 6th ed.* by Atkins et al.

Course Objectives. The primary objective of this course will be to introduce you to advanced covalent bonding theories, with primary emphasis on molecular orbital (MO) theory. MO theory provides a way of looking at bonding that is qualitatively different from the one conveyed by Lewis structures, and by simple valence bond ideas such as hybridization, with which you will be more familiar. Although you can get surprisingly far in inorganic chemistry using only simple tools such as Lewis structures, the MO view is absolutely essential for understanding inorganic spectroscopy (and indeed, spectroscopy in general). It also gives valuable insights into the nature of delocalized bonds, such as those found in many boron compounds, or in extended solids such as conductors and semiconductors.

These days, chemical problems of the sort amenable to MO theory are actually tackled using sophisticated computational packages that require an extensive math background to master them. In this course though, we will use a qualitative molecular orbital approach that takes advantage of any symmetry that a molecule might possess to greatly simplify things. The advantage of the qualitative approach is that it will allow us to explore a wide range of MO theory applications without getting bogged down in the mathematical details. Be advised though, that if you ever want to solve a real problem using the tools that we will learn about, you will probably first have to go back and learn about all the theoretical details that we skip here!

Prerequisites. This course will be easiest for you if you have previously done an introductory inorganic chemistry course such as Chem 311, and an introduction to quantum mechanics in a physical chemistry course such as Chem 562.

For those of you that haven't yet done quantum mechanics in P-chem I will do a brief review of the basics during the first week of class; this should be enough to get you through this course.

For those of you that have never done introductory inorganic chemistry, I have posted the following on D2L: (1) Parts 1-3 of my Chem 311 notes; (2) The Chem 311 syllabus, which lists the problem sets for the course; (3) Chapter 1 of the Chem 311 text book by Wulfsberg, which contains many of the recommended problems listed in the Chem 311 syllabus. ***I strongly recommend that, before class starts, you read through the posted material, and do the assignments that are marked as "hand-in" in Problem Sets 1-5***. Most of this is review of freshman chemistry; however, there are a few subtle but important additions. If you have any questions about this material let me know by email, or drop by my office.

Assignments. There will be no formal exams in this course. Instead, you will periodically hand in short assignments for grading. During the last week(s) of class you will also each give a Powerpoint presentation on a topic of your choice. You will need to choose an inorganic chemistry topic for your Powerpoint presentation by the first week of March at the latest. The presentation itself should be 20-30 min.

You are encouraged to use all the resources at your disposal when working on your assignments. These include the Shriver and Atkins text book, any other reference book or journal article, faculty members including me, and even your fellow students. I have no problem with many of you working together on your problems, ***but with one condition: you can discuss questions with other students in the class, prior to writing down your answers to the questions; however, you may not consult with other students while you are writing up your answers.*** Please be advised that it is very easy for me to tell if two or more students have collaborated in ***writing*** an answer. Each of you has a unique way of putting your thoughts on paper, and you cannot disguise it if you have copied the ideas from someone else! If two or more students collaborate in writing the answers to a problem set, all of the collaborators will receive a zero for that problem set.

2. Topics to be covered

i. Quantum mechanics (review/preview)
ii. Orbitals, terms and states
iii. Valence bond theory
iv. Molecular orbital theory, part 1
v. Symmetry and group theory
vi. Some simple applications of group theory
    identifying chiral compounds
    identifying molecules with a dipole moment
    infrared/Raman spectroscopy
vii. Molecular orbital theory, part 2
vii. Selected special topics

3. Suggested reading list

Recommended Text:

Atkins, P., Overton, T., Rourke, J., Weller, M., Armstrong, F., Hagerman, M. "Shriver and Atkins Inorganic Chemistry, 3rd - 6th edition"; W. H. Freeman and Co.
ISBN 0-7167-4878-9

Other Recommended Books

1. Wulfsberg, G. "Inorganic Chemistry"; University Science Books, 2000;
ISBN 1891389017; QD151.5.W84 2000

2. M. Gerloch "Orbitals, Terms and States"; John Wiley and Sons, 1986.

ISBN 0471909351 (cloth), 047190936X (paper); QD461.G37 1986

3. D. M. P. Mingos "Essential Trends in Inorganic Chemistry"; Oxford University Press, 1998. ISBN 0198501099; QD467.M64 1997

4. M. Gerloch, E. C. Constable "Transition Metal Chemistry, The Valence Shell in d-Block Chemistry"; VCH, 1994. ISBN 1560818840; QD172.T6 G47x 1994

5. F. A. Cotton, G. Wilkinson "Advanced inorganic chemistry : a comprehensive text, 5th edition"; J. Wiley and Sons, 1988. ISBN 0471849979; QD151.2 C68 1988

6. F. A. Cotton "Chemical Applications of Group Theory, 3rd edition"; J. Wiley and Sons, 1990. ISBN 0471510947 QD461.C65 1990

Recommended Review Journals

1. Science (Published by the American Association for the Advancement of Science) Q1.S354; (Free internet access from campus: http://www.sciencemag.org/).

2. Nature (Macmillan Publishers Ltd) Q1 .N2. (Free internet access from campus)

3. Chemical Reviews (Published by the American Chemical Society) QD1 .A5635; (Free internet access from campus: http://pubs.acs.org/journals/).

4. Accounts of Chemical Research (Published by the American Chemical Society) QD1.A31x (Free internet access from campus: http://pubs.acs.org/journals/).

5. Chemical and Engineering News (Published by the American Chemical Society) TP1.C35; ; (Free internet access from campus: http://pubs.acs.org/journals/). (Generally short articles, but good for ideas).

6. Scientific American (Scientific American, inc.) T1 S5 (Light reading, very general; covers all of science).

Recommended Primary Journals from the American Chemical Society (Free internet access from campus computers (http://pubs.acs.org/journals/):

1. Journal of the American Chemical Society (QD1.A5)

2. Inorganic Chemistry (QD1.I615)

3. Organometallics (QD410.O733)