

Syllabus for CHEM3120
Chemical Systems II
Winter Quarter 2007; revised 12/17/06
Professor G. R. Eaton

Description:

This course is described in the bulletin as follows: "Interpretation of the chemistry of the elements in terms of orbital interactions. Most examples will be taken from the 3d transition metals and the boron and carbon groups." Throughout, there will be an emphasis on periodic properties. Chemistry of the elements is a very broad field of study. To fit within a one-Quarter course, we will restrict our focus to emphasize molecular species, and usually small molecular species.

Goals

This course attempts to convey a qualitative and intuitive approach to overall trends in the periodic table. Using symmetry, shapes of atomic and molecular orbitals, electronegativity, effective nuclear charge, etc., you can describe many chemical phenomena and you can know whether you should be surprised by a new chemical observation. You do have to practice a lot to develop insight into what approximations you can make, and in what context they are useful. When you successfully complete this course, you should be able to understand at a useful level the chapters about periodicity and transition elements in a freshman chemistry text. It is hoped that with a solid foundation in discrete monomolecular species, you will be able to extrapolate to extended solids, nanomaterials, etc. Boron is included for two reasons: B has 3 valence electrons and 4 valence orbitals, resulting in structures and chemistry very different from that of C. We can extend the MO concepts you have learned in organic and physical chemistry to polyhedral B systems, still using only s and p orbitals. Then, we will see that the symmetries of the resultant MOs are the same as the symmetries we encounter when we expand the orbital basis set to include d orbitals for the transition elements in coordination compounds.

Background assumed:

This course will build upon your undergraduate education in descriptive chemistry of the elements, small amounts of introductory biochemistry, and some of the content of CHEM3310 (MS&E I). The treatment of atomic and molecular orbitals, symmetry, and group theory will follow on from where you left off in MS&E I. It will be assumed that you are taking CHEM3320 (MS&E II), which introduces computational methods in chemistry. The sequence of topics in CHEM 3120 will be coordinated with the sequence in CHEM3320. For example, we will present results of current computational chemistry of transition metal complexes, including comparison of DFT with LFT, based on the Gaussian calculations you will be learning how to do in MS&E II. Professor Kutateladze will accept computational projects in MS&E II that relate to the topics in CHEM 3120. One of your cooperative learning group problems will be to use what you learn in MS&E II to calculate one of the cases that we treat qualitatively in CHEM 3120, and to compare the quantitative and qualitative results. The timing of this assignment will be coordinated with MS&E II.

Text:

The text titled Inorganic Chemistry, Second Edition, 2005, by Catherine E. Housecroft and Alan G. Sharpe, Pearson Prentice Hall, ISBN 0130-39913-2, will be the primary text for this course. You should have learned in prior courses most of the material in the first half of this text. Texts commonly used in undergraduate study of the chemistry of the elements also will be valuable to you. A substantial amount of relevant chemistry is in the text by Silberberg, Chemistry: The Molecular Nature of Matter and Change, 4th ed., used in the general chemistry class at DU (1st ed. QD33.S576 1996). See, for example, chapter 8 on electron configuration and chemical periodicity, chapter 11 on properties of the elements, and chapter 23 on transition elements. For the study of symmetry and molecular orbitals you will find it useful to consult additional texts, such as the ones by Hall, Cotton, Carter, etc., that are listed at the end of this syllabus. References to original papers will be provided in class as topics are discussed.

Method of Instruction:

Instruction will be by assigned reading, homework problems, including some larger problems that you will solve in teams, and lectures. Lectures will assume that you have done the reading in advance, and will usually go beyond the material in the assigned readings. Reading in the text book is an alternate, additional, source of information, which will provide essential background to the material presented in lectures. Students are encouraged to work together to learn the material. Understanding of the material taught via homework problems will be sampled via short quizzes. Group cooperative learning projects will be graded. Everyone in the group will receive the grade of the group, modified by student assessments of relative contributions.

Schedule:

Class will meet MWF 10:00-10:50, in Olin 103. A tentative schedule is presented below. Classes start on Wednesday, January 3. Monday, January 15, is MLK Day. The last day of classes is Monday, March 12. Note that the final exam may not be at the time specified on the Registrar's schedule. It may be moved to avoid having it on the same day as the exam for another graduate core class, if requested by the class. Office hours are Tuesday, Wednesday, and Thursday 5-6 pm, or by appointment.

Tentative course outline and approximate schedule

class	Date	Topic	Reading [#]
1	W 1/3	Introduction to the course of study; Periodicity, Elements and Their Physical Properties; Oxides of the elements	Ch. 1, 5, 15, and Ch. 9 in Rayner-Canham or Rodgers
2	F 1/5	“	“
3	M 1/8	“	“
4	W 1/10	“	“
5	F 1/12	Multicenter bonding; The nature of solids; Lattice energies and solubility	Ch. 4, 5, 27
6	W 1/17	Symmetry, character tables; representations	Ch. 3, other texts on symmetry and group theory
7	F 1/19	Molecular orbitals as representations	”
8	M 1/22	Vibrations as representations	“
9	W 1/24	Coordination Complexes, Isomers	Ch. 19
10	F 1/26	Hydrides and alkyl compounds	Ch. 4, 12
11	M 1/29	“	“
12	W 1/31	MOs of metal complexes	Ch. 20
13	F 2/2	Electronic structure of metal complexes	“
14	M 2/5	“	“
15	W 2/7	“	“
16	F 2/9	Excited electronic states, Tanabe-Sugano diagrams, etc.	“
17	M 2/12	“	“
18	W 2/14	“	“
19	F 2/16	Exam (through lecture 15)	
20	M 2/19	Descriptive Chemistry of the Transition Elements	Ch. 21, 28
21	W 2/21	“	“
22	F 2/23	“	“
23	M 2/26	Reaction mechanisms	Ch. 25
24	W 2/28	“	“
25	F 3/2	“	“
26	M 3/5	“	“
27	W 3/7	Organometallic compounds and catalysis	Ch. 23, 26
28	F 3/9	“	“
29	M 3/12	Survey of Chemistry of the 2 nd and 3 rd row elements and the Lanthanides	Ch. 22, 24
		Final exam	

[#] Note that the Housecroft book has a very detailed table of contents and index via which you can locate additional pages of the text appropriate to each of the topics. For example, there is a section on periodicity, bond energies, etc., in each of the chapters that discuss groups of elements.

Grading

Group projects 20%

Quizzes 20%

Midterm exam 30%

Final exam 30%

The background material assumed for this course can be found in books such as:

If the library copy is checked out, ask others in the class before recalling the book.

Rodgers, Glen E., Introduction to Coordination, Solid State, and Descriptive Inorganic Chemistry. McGraw-Hill, 1994 QD474.R63 1994

Rodgers, Glen E., Descriptive inorganic, coordination, and solid state chemistry Brooks/Cole, 2002, 2nd ed. QD474 .R62 2002 The periodic tables and graphical illustrations of discovery of the elements are worth your study.

Rayner-Canham, Geoffrey, and Tina Overton, 2002. Descriptive Inorganic Chemistry, 3rd ed., W.H. Freeman, New York, QD151.5 .R39 2003 (2nd ed 2000 QD151.5 .R39 2000; 1st ed., 1996 QD151.5.R39 1996). Acquisition of the 4th edition has been requested. This is the text that has been used recently in CHEM 2130.

F. Albert Cotton, Geoffrey Wilkinson, Paul L. Gaus, Basic Inorganic Chemistry, 3rd ed. New York, J. Wiley, 1995. QD151.2.C69 1995

For molecular symmetry and group theory, you may find useful information in:

R. L. Carter, Molecular Symmetry and Group Theory. Wiley, New York, 1998. QD461.C32.1998 Many students have said that they like this text.

F. A. Cotton, Chemical Applications of Group Theory, 3rd ed., Wiley, New York, 1990. QD461.C65 1990 This is the “standard” reference in this field.

L. H. Hall, Group Theory and Symmetry in Chemistry. McGraw-Hill Book Co. New York, 1969. QD461.H17 I tend to use the notation of this book.

Web sites

It is very difficult to figure out whether a web site contains reliable information and whether it is up to date. The following web sites were selected as potentially useful or potentially interesting to you (sites were accessed on 11/27/06 and 12/11/06).

Note that the text has a web site: www.pearsoned.co.uk/housecroft that includes exercises for you to try, rotatable 3D structures for those so designated in the text, and an interactive periodic table. You will need the program “chime” to rotate the structures.

Web sites for Periodic Tables and Properties of the Elements

There are some other good web sites for sources of information about the elements:

www.webelements.com This site has been developed over a long time, and appears to have been prepared with care.

A searchable table, with links to many other sites, is available at <http://chemlab.pc.maricopa.edu/periodic/> The links in this table did not work on 12/17/05

The American Chemical Society web site has a periodic table that provides plots of various physical properties.
http://www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=sitertools%5Cperiodic_table.html#

Another useful site is www.chemicool.com/

An artistic interpretation of the elements is at www.chemsoc.org/viselements/
This site usually is very slow, and it is best viewed in a darkened room or with a very bright screen, since the artist used a lot of dark colors.

The Los Alamos National Lab periodic table provides historical, application, and financial information about each element. It has the advantage that you can download a pdf file and have it on your own computer. This pdf file lacks some of the colorful interactive aspects of the on-line version. This site uses a lot of dark backgrounds, white on black for text, etc.
<http://pearl1.lanl.gov/periodic/default.htm>

NIST has a very nice periodic table in pdf and tif formats, and data on each element:
<http://physics.nist.gov/PhysRefData/PerTable/index.html>
<http://physics.nist.gov/PhysRefData/contents.html>

If you would like a nice, colorful, periodic table, look at
<http://www.theodoregray.com/PeriodicTable/Posters/index.html>

For a little entertainment, try web sites for the song "the elements" by Tom Lehrer
<http://www.casualhacker.net/tom.lehrer/evening.html#elements>

<http://www.privatehand.com/flash/elements.html>

Web sites for symmetry:

<http://www.phys.ncl.ac.uk/staff/njpg/symmetry/>
this site gives pictures that rotate so the molecules can be seen from many directions, and some nice pictures of stereographic projections with molecules

<http://www.ch.ic.ac.uk/vchemlab/symmetry/>
this site needs chime to show modes in action

<http://www.reciprocalnet.org/edumodules/symmetry/>
this site has a good tutorial with pictures of planes and axes, etc.

<http://csi.chemie.tu-darmstadt.de/ak/immell/index.html> click on tutorials, which include symmetry, atomic orbitals, chirality, and other topics.

See Journal of Chemical Education, November 2005, page 1736 and 1741. These articles tell of using Jmol and WebWare for learning molecular symmetry.

<http://0-jchemed.chem.wisc.edu.bianca.penlib.du.edu/JCEDLib/WebWare/collection/reviewed/JCE2005p1742WW/jcesubscriber/symmetry/index.htm>

http://0-jchemed.chem.wisc.edu.bianca.penlib.du.edu/JCEDLib/WebWare/collection/reviewed/JCE2005p1741_2WW/jcesubscriber/3DMolSym/Index.htm

Mechanisms that Interchange Axial and Equatorial Atoms in Fluxional processes: Illustration of the Berry Pseudorotation, the Turnstile and the Lever Mechanisms via animation of transition state normal vibrational modes. Marion Cass, King Kuok (Mimi) Hii and Henry S. Rzepa J. Chem. Ed. 83(2) 336 (2006) and the on-line movies of atom motion.

Links to other chemical information

The Royal Society of Chemistry (www.chemsoc.org) and the American Chemical (www.chemistry.org) Society provide links to many sources of chemical information.

The following web site gives a time line for major events in science:

<http://www.chemsoc.org/timeline/pages/timeline.html>