CHEM3120
Chemical Systems II
Winter Quarter 2006; revised 01/01/06
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 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.

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 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.

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. 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. Some of these additional texts are listed at the end of this syllabus. References to original papers will be provided in class as topics are discussed. A list of additional sources of information that you may find useful will be given to you from time to time.

Method of Instruction:

Instruction will be by assigned reading, homework problems, including some larger problems that you will solve in teams, and lectures. Reading in the text book is an alternate, additional, source of information, which will provide essential background to the material presented in lectures. Lectures will assume that you have done the reading in advance, and will usually go beyond the material in the assigned readings. Students are encouraged to work together to learn the material. Homework will not be graded. Instead, the 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 9:00-9:50, in Olin 103. A tentative schedule is presented below. 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.

Classes start on Wednesday, January 4. Monday, January 16, is MLK Day. The last day of classes is Tuesday, March 14.

Tentative course outline and approximate schedule

class	Date	Topic	Reading#
1	W 1/4	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 1/6	"	"
3	M 1/9	"	"
4	W 1/11	"	"
5	F 1/13	Multicenter bonding; The nature of solids; Lattice energies and solubility	Ch. 4, 5, 27
6	W 1/18	Symmetry, character tables; representations	Ch. 3, other texts on symmetry and group theory
7	F 1/20	Molecular orbitals as representations	"
8	M 1/23	Vibrations as representations	"
9	W 1/25	Coordination Complexes, Isomers	Ch. 19
10	F 1/27	Hydrides and alkyl compounds	Ch. 4, 12
11	M 1/30	"	"
12	W 2/1	MOs of metal complexes	Ch. 20, extensively supplemented in lectures
13	F 2/3	Electronic structure of metal complexes	"
14	M 2/6	"	"
15	W 2/8	"	"
16	F 2/10	Excited electronic states, Tanabe-Sugano diagrams, etc.	"
17	M 2/13	"	"
18	W 2/15	"	"
19	F 2/17	Exam (through lecture 15)	
20	M 2/20	Descriptive Chemistry of the Transition Elements	Ch. 21, 28
21	W 2/22	"	"
22	F 2/24	"	"
23	M 2/27	Reaction mechanisms	Ch. 25
24	W 3/1	"	"
25	F 3/3	"	"
26	M 3/6	"	"
27	W 3/8	Organometallic compounds and catalysis	Ch. 23, 26

28	F 3/10	"	"
29	M 3/13	Survey of Chemistry of the 2nd and 3rd row elements and the Lanthanides	Ch. 22, 24
	W 3/15	Final exam	8:00-9:45

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.

Bibliography of potentially useful books.
If the library copy is checked out, ask others in the class or me before recalling the book.

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

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

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).

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

When searching for specific aspects of chemistry covered in this course, you may find it useful to refer to one of the other text books that have been used in this course in prior years, or could be used in this course.

Keith F. Purcell, John C. Kotz, Inorganic chemistry, Philadelphia, Saunders, 1977. QD151.2.P87

Bodie E. Douglas, Darl H. McDaniel, John J. Alexander, Concepts and models of inorganic chemistry, 3rd ed., New York: Wiley, c1994. QD475.D65 1994

Duward F. Shriver, Peter Atkins, Cooper H. Langford, Inorganic Chemistry, 2nd ed., New York : W.H. Freeman, 1994. QD151.5.S57 1994

Duward F. Shriver and Peter Atkins, Inorganic Chemistry, 3rd ed., New York: W.H. Freeman, 1999. QD151.5 .S57 1999

G. L. Meissler and D. A. Tarr, Inorganic Chemistry, 3rd ed., Prentice-Hall, Englewood Cliffs, NJ, 2004. second edition: QD151.2 .M54 1999

G. Wulfsberg, Inorganic Chemistry, University Science Books, Sausalito, CA, 2000. QD151.5 .W84 2000

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

F. A. Cotton, Chemical Applications of Group Theory, 3rd ed., Wiley, New York, 1990. QD461.C65 1990

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.

I commonly refer to the following books:

N.N. Greenwood and A. Earnshaw, Chemistry of the elements. 2nd ed. Butterworth-Heinemann, Oxford, Boston, 1997. QD466 .G74 1997

F. Albert Cotton ... [et al.] ; with a chapter on boron by Russell Grimes. Advanced Inorganic Chemistry. 6th ed., New York, Wiley, 1999, QD151.2 .C68 1999, or prior editions.

Inorganic chemistry / founded by A.F. Holleman ; continued by Egon Wiberg ; translated by Mary Eagleson, William Brewer ; revised by Bernhard J. Aylett. 1st English ed., edited by Nils Wiberg., Academic Press ; San Diego, Berlin, New York : De Gruyter, 2001. QD151.3 .W5313 2001

A.B.P. Lever, Inorganic electronic spectroscopy, 2nd ed., Elsevier, Amsterdam, New York, 1984. QD96.E44 L49 1984

T. Schönherr, Optical Spectra and Chemical Bonding in Inorganic Compounds. Structure and Bonding, Volume 106. Springer, Berlin, 2004. QD461.S92.v.106

D. H. Rouvray and R. B. King, eds. The Periodic Table: Into the 21st Century. Research Studies Press Ltd. Hertfordshire, England, Institute of Physics Publishing.2004. QD467.P4756 2004 History and structure of the periodic table.

Additional information may be found in one of the comprehensive treatises on inorganic chemistry.

Comprehensive coordination chemistry: the synthesis, reactions, properties and applications of coordination compounds, 1st ed., editor, Sir Geoffrey Wilkinson, executive editors, Robert D. Gillard, Jon A. McCleverty, Oxford, England ; New York : Pergamon Press, 1987. Reference Stacks QD474 .C65 1987

Comprehensive inorganic chemistry. Editorial board: J. C. Bailar, Jr., H. J. Emeléus, Sir Ronald Nyholm [and] A. F. Trotman-Dickenson (executive editor) Pergamon Press; distributed by Compendium Publishers, Elmsford, N.Y., 1973 QD151.2.C64

Comprehensive Organometallic Chemistry : the synthesis, reactions, and structures of organometallic compounds, editor, Sir Geoffrey Wilkinson ; deputy editor, F. Gordon A. Stone ; executive editor, Edward W. Abel, Oxford, [Oxfordshire] ; New York : Pergamon Press, 1982. Reference Stacks QD411.C66 1996

Comprehensive organometallic chemistry II: a review of the literature 1982-1994, editors-in-chief, Edward W. Abel, F. Gordon A. Stone, Geoffrey Wilkinson, Oxford; New York: Pergamon, 1995. Reference Stacks QD411.C652 1995

Comprehensive Supramolecular Chemistry, J. L. Atwood et al., eds., Oxford, Pergamon, 1996. QD411.C66 1996 This is an update of Comprehensive Organometallic Chemistry, 1982.

Dictionary of inorganic compounds, executive editor, J.E. Macintyre ; assistant editors, F.M. Daniel, V.M. Stirling,. London; New York: Chapman & Hall, 1992. Reference Stacks QD148.D538 1992

Encyclopedia of inorganic chemistry / editor-in-chief, R. Bruce King, Chichester; New York: Wiley, 1994. Reference Stacks QD148.E53 1994

Encyclopedia of computational chemistry / editor-in-chief, Paul von Ragué Schleyer, 1998 Reference Stacks QD39.3.E46 E53 1998

The porphyrin handbook / editors, Karl M. Kadish, Kevin M. Smith, Roger Guilard, volumes 1-10, 2000 Reference Stacks QD401 .P824 2000

WWW Web sites were accessed on 12/17/05.
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 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

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

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/immel/index.html click on tutorials, which include symmetry, atomic orbitals, chirality, and other topics.

See Journal of Chemical Education, November 2005, page1736 and 1741. These articles tell of using Jmol and WebWare for learning molecular symmetry.