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**

<table>
<thead>
<tr>
<th>Class</th>
<th>Date</th>
<th>Topic</th>
<th>Reading</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>W 1/4</td>
<td>Introduction to the course of study; Periodicity, Elements and Their Physical Properties; Oxides of the elements</td>
<td>Ch. 1, 5, 15, and Ch. 9 in Rayner-Canham or Rodgers</td>
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<td>2</td>
<td>F 1/6</td>
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<td>3</td>
<td>M 1/9</td>
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<td>4</td>
<td>W 1/11</td>
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<tr>
<td>5</td>
<td>F 1/13</td>
<td>Multicenter bonding; The nature of solids; Lattice energies and solubility</td>
<td>Ch. 4, 5, 27</td>
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<tr>
<td>6</td>
<td>W 1/18</td>
<td>Symmetry, character tables; representations</td>
<td>Ch. 3, other texts on symmetry and group theory</td>
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<tr>
<td>7</td>
<td>F 1/20</td>
<td>Molecular orbitals as representations</td>
<td>“</td>
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<tr>
<td>8</td>
<td>M 1/23</td>
<td>Vibrations as representations</td>
<td>“</td>
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<tr>
<td>9</td>
<td>W 1/25</td>
<td>Coordination Complexes, Isomers</td>
<td>Ch. 19</td>
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<td>10</td>
<td>F 1/27</td>
<td>Hydrides and alkyl compounds</td>
<td>Ch. 4, 12</td>
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<td>11</td>
<td>M 1/30</td>
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<tr>
<td>12</td>
<td>W 2/1</td>
<td>MOs of metal complexes</td>
<td>Ch. 20, extensively supplemented in lectures</td>
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<tr>
<td>13</td>
<td>F 2/3</td>
<td>Electronic structure of metal complexes</td>
<td>“</td>
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<tr>
<td>14</td>
<td>M 2/6</td>
<td>“</td>
<td>“</td>
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<tr>
<td>15</td>
<td>W 2/8</td>
<td>“</td>
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<tr>
<td>16</td>
<td>F 2/10</td>
<td>Excited electronic states, Tanabe-Sugano diagrams, etc.</td>
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<tr>
<td>17</td>
<td>M 2/13</td>
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<tr>
<td>18</td>
<td>W 2/15</td>
<td>“</td>
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<tr>
<td>19</td>
<td>F 2/17</td>
<td>Exam (through lecture 15)</td>
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<tr>
<td>20</td>
<td>M 2/20</td>
<td>Descriptive Chemistry of the Transition Elements</td>
<td>Ch. 21, 28</td>
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<tr>
<td>21</td>
<td>W 2/22</td>
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<td>22</td>
<td>F 2/24</td>
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<td>23</td>
<td>M 2/27</td>
<td>Reaction mechanisms</td>
<td>Ch. 25</td>
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<td>24</td>
<td>W 3/1</td>
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<td>25</td>
<td>F 3/3</td>
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<tr>
<td>26</td>
<td>M 3/6</td>
<td>“</td>
<td>“</td>
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<tr>
<td>27</td>
<td>W 3/8</td>
<td>Organometallic compounds and catalysis</td>
<td>Ch. 23, 26</td>
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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:


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.


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


I commonly refer to the following books:


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


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.chemicoool.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/njpj/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.