

Chemical Information Retrieval (CHEM367 - Meets at the same time and place as CHEM767)

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Office hours Tu & Th 17:00-18:00, also by appointment or drop-in.

Where: Pearlstein Business Center 206

When: Fall term 2016, F 16:00-18:50

Text: none.

The purpose of this class is to help students of chemistry, (and related disciplines) build skills in locating chemical and related scientific information. Objectives are:

- to secure a basic grasp of the chemical literature and its derived electronic databases
- to develop insight into the cost and value of chemical information
- to develop a basic skills in locating relevant and high quality chemical information
- to gain basic experience in the scientific writing process

Grading: There will be four components to the course grade.

- 1) database construction (team project), 20%
- 2) in-class exam, 20%
- 3) paper, 45%
- 4) In-class activities and instructor's discretionary component, 15%.

The final letter grade for the course will be determined according to the following scale:

90.00-92.99, 93.00-97.99, 98.00-100 are A-, A, A+, respectively.

80.00-82.99, 83.00-86.99, 87.00-89.99 are B-, B, B+, respectively.

70.00-72.99, 73.00-76.99, 77.00-79.99 are C-, C, C+, respectively.

0.00-59.99, 60.00-66.99, 67.00-69.99 are F, D, D+, respectively.

The instructor reserves the right to lower, but not raise, the letter grade thresholds, but in no case will a score of less than 50% result in a passing grade for the class.

Attendance is expected and may influence the "instructor's discretionary component" of the final letter grades.

Adherence to university computer usage policy is expected. Violations of this policy will be dealt with at the greatest level of severity allowed under university policy.

Additional resources:

- Academic policies: <http://www.drexel.edu/provost/policies/overview/>
- Disability resources: <http://www.drexel.edu/oed/disabilityResources/overview/>
- Information resources: <http://drexel.edu/irt/news/publications/itgblog/>
- Library website: <https://www.library.drexel.edu/>
- Student handbook: http://drexel.edu/studentaffairs/community_standards/studentHandbook/

Course schedule (Approximate and subject to change)

- 9/23 (Discussion of syllabus and assignments)
 - spin coupling & term symbols as motivation for accurate data tabulation
(<http://web.chem.ucsb.edu/~devries/chem218/termsymbols.pdf>)
(<http://web.chem.ucsb.edu/~devries/chem218/Term%20symbols.pdf>)
 - Charlotte Moore's tables (<https://www.nist.gov/srd/srd-publications/national-standard-reference-data-series-nsrds>)
 - assignment of database project.
 - assignment of "contents" project for CHEM367 students.
 - assignment of review paper for CHEM767 students. (367 may substitute this.)
 - classroom activity: database team organization.
- 9/30 (Traditional handbooks and indexes)
 - Physical and chemical properties
 - CRC handbook (<http://www.hbcnetbase.com/>)
 - (<http://www.library.drexel.edu/cgi-bin/r.cgi?url=http://www.hbcnetbase.com/>)
 - Merck Index (<https://www.rsc.org/Merck-Index/>)
 - (<http://www.library.drexel.edu/cgi-bin/r.cgi?url=https://www.rsc.org/Merck-Index/>)
 - WebElements (<http://www.webelements.com/>)
 - Crystal structures:
 - American Mineralogist Crystal Structure Database (<http://rruff.geo.arizona.edu/AMS/amcsd.php>)
 - Mineralogy database (<http://webmineral.com/>)
 - Russian foundation crystallographic database (<http://database.iem.ac.ru/mincryst/>)
 - Crystallography Open Database (<http://www.crystallography.net/>)
 - A for-pay crystal structures database (<http://icsd.fiz-karlsruhe.de/>).
 - review Hess' Law and thermochemical cycles.
(<https://www.khanacademy.org/science/physics/thermodynamics/v/hess-s-law-example>)
 - JANAF thermochemical tables
 - (<http://kinetics.nist.gov/janaf/>)
 - (<http://catalog.data.gov/dataset/nist-janaf-thermochemical-tables-srd-13>)
 - (<https://www.nist.gov/srd/journal-physical-and-chemical-reference-data-monographs-or-supplements>)
 - Toxicology and safety information
 - MSDS
 - ChemSpider (<http://www.chemspider.com/>)

- US Department of Health and Human Services household products index (<http://householdproducts.nlm.nih.gov/index.htm>)
 - FDA approved drug products: (http://www.accessdata.fda.gov/scripts/cder/drugsatfda/index.cfm?fuseaction=Search.Search_Drug_Name)
 - NIH database dietary supplement label database: (<http://www.dsld.nlm.nih.gov/dsld/>)
 - classroom activity: Hess' Law challenge
- 10/7 (The scientific literature, what it is and how to find it)
 - Peer review: what, how, why (<http://science.howstuffworks.com/innovation/scientific-experiments/scientific-peer-review.htm>)
 - Science Citation Index
 - tutorials: (http://wokinfo.com/training_support/training/web-of-science/)
 - Impact factor
 - h-index
 - Google Scholar (<http://scholar.google.com/>)
 - tutorial: (<https://www.youtube.com/watch?v=t1ZwgDeX2eQ>)
 - PubChem (<http://pubchem.ncbi.nlm.nih.gov/>)
 - FPO (<http://www.freepatentsonline.com/>)
 - classroom activity: searching activity
- 10/14 (Guest speaker from library)
 - Resources available from library
 - ILLiad
 - electronic resources
 - human resources
 - search engines to databases
- 10/21 (A prescription for writing)
 - Who did what?
 - Turn 10 key points into 10 sentences.
 - Build a case to support each key point.
 - Summarize
 - Use EndNote - (Often you can obtain references in EndNote format from the SCI or journal web sites)
 - Am I sure it is my own work? (<http://www.ithenticate.com/>)
 - Types of plagiarism: http://www.turnitin.com/assets/en_us/media/plagiarism_spectrum.php
- 10/28 (Finding scientific papers and managing references, Guest speaker from library)
 - SciFinder Scholar - (Chemical Abstracts searching)
 - EndNote
- 11/4 (ACS guidelines and professionalism)

- discussions of examples in, "On being a Scientist"
 - The Flint water crisis.
 - discussions of other readings
- 11/11 (Guest speaker from Technology Commercialization)
 - Patents, Intellectual Property and Technology Commercialization.
- 11/18
 - in-class test
- 12/2 (Resources for solving mathematical problems)
 - CRC Standard Mathematical Tables (<http://www.mathtable.com/smtf/>)
 - Handbook of Mathematical Functions (Abramowitz & Stegun)
(http://people.math.sfu.ca/~cbm/aands/abramowitz_and_stegun.pdf)
 - review Interpolation from tables
 - Table of Integrals, Series, and Products (Gradshteyn & Ryzhik)
(<http://www.mathtable.com/gr/>)
 - Review u-substitution
 - Software tools: (Maple, Mathematica)
 - Wolfram alpha (<http://www.wolframalpha.com/>)
 - classroom activity: interpolation and integration

All links functional as of 09/08/2016