Finding inorganic chemical information

Library session for Chemistry 108
Inorganic Synthesis Laboratory
Fall 2010

Chemistry & Chemical Engineering Library
University of California, Berkeley

Outline of learning activities

1. Understand how this class may help

By the end of the class, you will be able to find chemical information to supplement your lab reports on inorganic syntheses. These skills will help with scientific writing as well as grade maximization.

For specific learning objectives, please review the outline of learning activities beginning on page 2.

2. Icebreaker

My classmate's name is _____

His/her high school mascot was _____

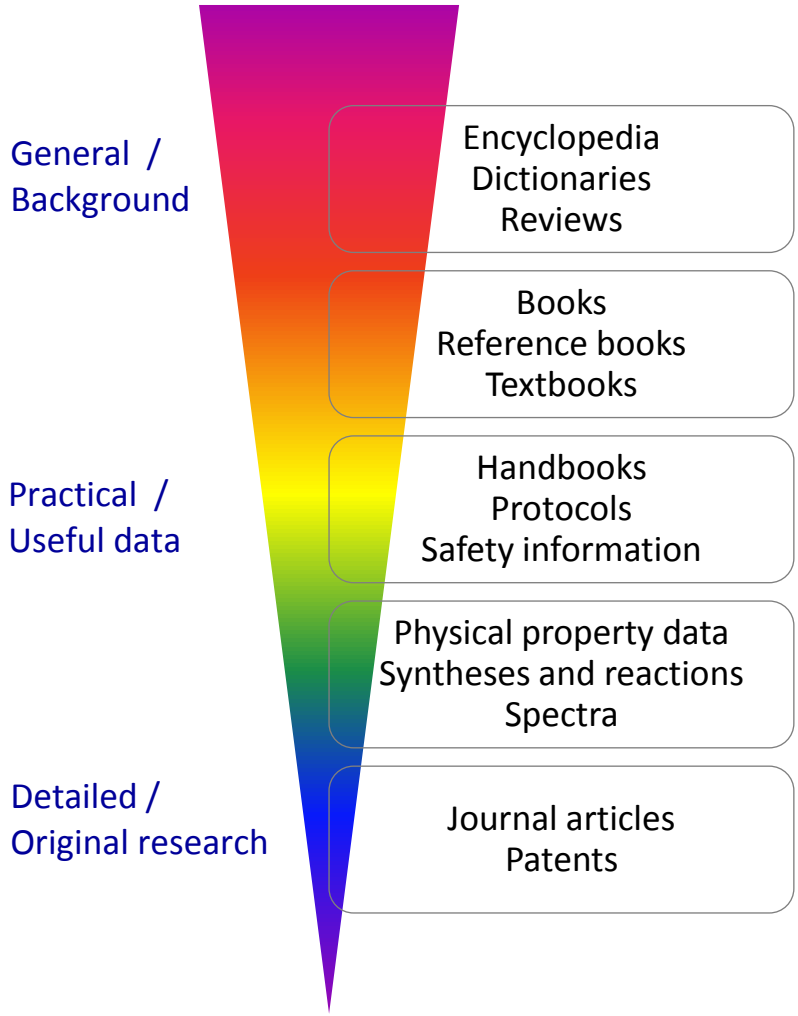
His/her favorite thing about Cal is _____

S/he recommends this book, song, movie, sport, hobby, television show, etc. (***pick one***) for Chemistry 108 classmates:

_____

3. Categorize chemical information resources by type of information, source types, and how they may be useful

Figure 1. Chemical information resources organized by purpose (left) and type of information (right)



The following guide gives examples of chemical information sources with recommendations.
http://units.sla.org/division/dche/il/cheminfolit.pdf

Resources can also be grouped by primary, secondary, and tertiary resources.

Information resource type	Example	Focus	Currency of information
Tertiary	Encyclopedia Databases Handbooks Textbooks	Topic overview, explanation, instruction, or history	Takes a long time to publish – therefore, not always current
Secondary	Review articles Annual reviews	Reviews the current state of knowledge Focus may vary (can resemble a tertiary or a primary resource)	Currency may vary (can resemble a tertiary or a primary resource)
Primary	Journal article	Detailed accounts of experiments and results by the researcher	At the time of publication, journal articles represent current research

The different parts of a journal article give you different types of information.

- **Introduction / background** provides an overview of the research topic or its history
- **Methods** explain the experimental protocols and techniques
- **Results** provide findings, numerical values, etc.
- **Discussion** explains the findings and explores how the results relate to broader themes and ideas
- **Conclusions / future research** summarize the study and identify next steps for further exploration

4. Use information resources and data in scientific writing

4.1. Know when to use information resources in scientific and lab report writing

Show key/foundational/seminal articles about the topic to help:

- understand the history of the topic
- identify the first synthesis

Collect background information to understand:

- what is already known about your topic
- how your research is unique and contributes to the knowledge base
- the importance of the topic
- how you are building your research in light of an established knowledge base, technique, or tradition

Compare your results with similar compounds, similar systems, or other researchers' findings – for example:

- confirm your findings with others
- identify differences between your findings and others
- compare to theoretical predictions and values

Justify and explain your ideas or generalizations

- demonstrate how your research findings fit or do not fit with others' findings
- show similarities between your research and others'

Describe the general direction or the future of a research topic by analyzing others' research experiences

Find tools and resources that you used in your research or for your research interpretation – such as models, theories, data, techniques, lab manuals, etc.

Resolve problems or challenges encountered in research

- learn tips and suggestions from other scientists' research
- identify solutions and new techniques

4.2. After using an information resource in your writing, prepare citations

4.2.1. Why?

Citations are a way of giving credit to information resources that you used.

If you use an information resource, you need to make a citation in your report to:

- avoid plagiarism and show the reader that you used information from another source (e.g., ideas, knowledge, or data that are not your own)
- help readers find resources to learn more about the topic

4.2.2. How to prepare citations

Here is a **sample citation** in the ACS style for a journal article.

1. Evans, D. A.; Fitch, D. M.; Smith, T. E.; Cee, V. J. Application of Complex Aldol Reactions to the Total Synthesis of Phorboxazole B. *J. Am. Chem. Soc.* **2000,** 122, 10033-10046.

You put the above citation in the references section of your paper or lab report (typically at the end).

In the body of your paper, you **cite references next to the idea or information you used** from a resource. You mark them with a footnote or with italic numbers in parentheses like below (among other options).

- Oscillation in the reaction of benzaldehyde with oxygen was reported previously.[3]
- The mineralization of TCE by a pure culture of a methane-oxidizing organism has been reported (*6*).

(Examples are from the ACS Style Guide, 3rd edition).

Tips

- Penn State University Libraries has a quick guide to the ACS citation style: http://www.libraries.psu.edu/content/dam/psul/up/pams/documents/QuickGuideACS.pdf
- Journal titles are abbreviated in ACS style citations. Find abbreviations with CASSI: http://cassi.cas.org/
- Here is a detailed chapter from the ACS Style Guide on preparing citations: http://pubs.acs.org/userimages/ContentEditor/1246030496632/chapter14.pdf

5. Use a tertiary resource to find background information for an inorganic chemical

5.1. Draw a structure to search an online chemical dictionary

Let's search the **Combined Chemical Dictionary** for an inorganic compound.

1. Visit http://www.lib.berkeley.edu/CHEM/
2. Select *Electronic Books*
3. Select *Combined Chemical Dictionary*
4. To search for hexamethyldisiloxane (HMDSO) by chemical structure:
    a. Firstly, draft the chemical structure.

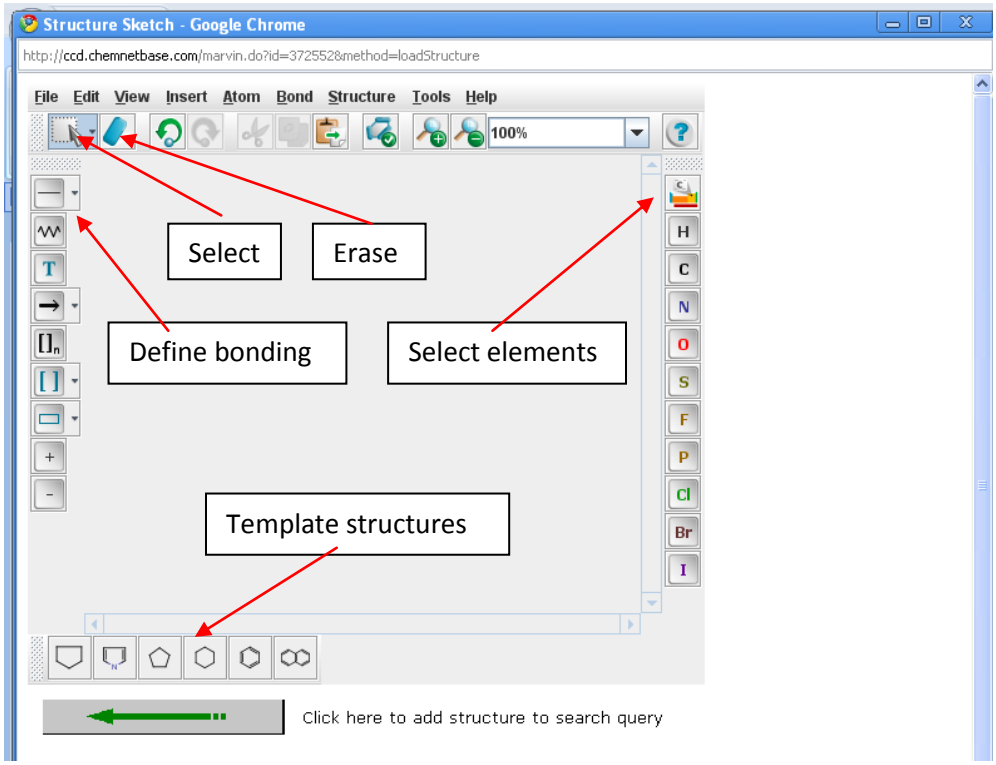
    In the box below, draw HMDSO using the conventions of skeletal structures for organic compounds (i.e. stick diagrams with implicit hydrogens).

    $Me_3Si–O–SiMe_3$

    
    Please pause for class discussion.

    b. Return to the search menu of Combined Chemical Dictionary and click *Draw Query*.
    c. Draw the structure you sketched above. Here are some tips:
        i. Skip hydrogens.
        ii. With carbons, follow the conventions of skeletal structures for organic compounds. Simply draw a line to indicate a carbon or carbon chain.
        iii. Draw the elements and functional groups and then link them together with the appropriate bond.

iv. To draw a chemical bond, select the bond type and then draw a line between the elements and functional groups.



d. When you're done drawing, click the *green arrow* at the bottom.

e. Now you're back at the main search page (with your structure in the search box). In the *Structure Matching* menu, select *substructure*.

f. Click search.

5. How many results do you find when you conduct a substructure search? _____

6. Randomly, select a result and view the chemical structure. Open and view a few more.

7. Think about the structures you viewed and compare them to the structure you drew originally (HMDSO). Is there a pattern? (In other words, how are these compounds related to your original structure?)

_____

_____

_____

_____

_____ _____

8. What do you think a substructure search is doing? Think sub and structure.

_____

_____

_____

_____

 Please pause for class discussion.

9. From the search results page, click *Return to Search*. Your structure should be in the query box. If it's missing, redraw the structure.
10. In the *Structure Matching* menu, select *Exact Match*.
11. View record for Hexamethyldisiloxane.
    a. What is HMDSO's molecular weight? _____
    b. What is one of its synthetic uses?

       _____

    c. Record a reference article that provide the Si-29 NMR spectra for HMDSO

       _____

       _____

    d. How is HMDSO synthesized?

       _____

       _____ _____
12. Now that you have used a tertiary chemical information resource, what do you think you will use it for?

_____

_____

_____

_____

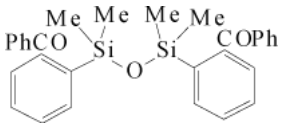
 Please pause for class discussion.

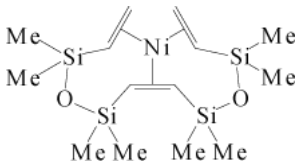
5.2. Post-activity discussion

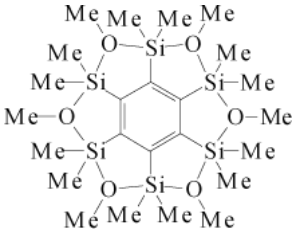
- Different databases and e-resources can have **different systems for drawing chemical structures**

- Substructure versus exact structure searching
    - **Exact structure searching** retrieves compounds with the exact same elements and connectivity as drawn or represented
    - **Substructure searching** retrieves compounds that have within its structure the same elements and connectivity as the query (ignoring hydrogens)
        - In other words, if you conduct a substructure search for a chemical fragment or pattern, it will retrieve molecules that contain that fragment or pattern.

          For example, a substructure search for Me3Si–O–SiMe3 retrieves:





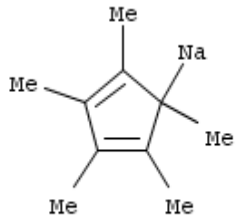


- Use tertiary resources like encyclopedia, textbooks, dictionaries, to find:
    - Background details
    - Basic chemical properties and values
    - Descriptions of the chemical and its uses
    - References to further information sources
    - Resources that report the first syntheses
    - And more …

6. Search by molecular formula

6.1. DEMONSTRATION: Sometimes chemical structure searching does not work

1. In the Combined Chemical Dictionary, perform a structure search for sodium Cp* (Cp* = pentamethylcyclopentadiene).



2. No records retrieved – even though the structure is drawn correctly. The search did not recognize the structure drawn.
3. Try a chemical name search for sodium pentamethylcyclopentadiene. Again, no results. The search did not retrieve a record by chemical name.
4. Let's try searching by molecular formula.

Molecular formula searching

When do use molecular formula searching?

- When drawing a chemical structure is complex, or
- When databases don't recognize the chemical structure you drew or the chemical name you typed

When searching, write your molecular formulae using the **Hill system order**

1. Write the *carbon* count first
2. Next, write the *hydrogen* count
3. Then, in alphabetical order of the *remaining elements* and their count

* *Do not include the number if the count is 1.*

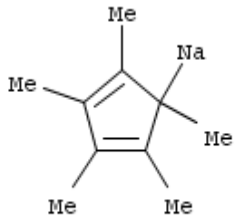
If the compound **does not contain carbon**, then write all the elements (and their count) in alphabetical order, including hydrogen.

Examples of molecular formulas in Hill order

CH3I
C2H5Br
H2O4S
BrH
BrI

6.2. Searching for Sodium Cp* by molecular formula

Let's search by molecular formula for sodium Cp*:



1. Write the molecular formula for sodium Cp* in Hill system order.
    a. First, what is the carbon count? _____
    b. What is the hydrogen count? _____
    c. What is the remaining element and its count? _____
    d. With the above data, write the molecular formula for sodium cp* in Hill order

    _____
2. In the Combined Chemical dictionary, start a new search by clicking *Search* in the upper left hand corner.
3. In the molecular formula property search box, enter the Hill order molecular formula for sodium Cp*.
    a. What is the CAS Registry Number for sodium Cp*? _____
    - Name a derivative of sodium Cp* _____
    - Is this derivative a solid, liquid, or gas? _____


Please pause for class discussion.

6.3. Post-activity discussion

- If searching by chemical structure or chemical name does not work, search by molecular formula in Hill order.
- Boolean operators help you search across different types of information and combine them appropriately:
    - AND = searches for all terms and conditions listed
    - OR = searches for either terms and conditions listed
    - NOT = excludes the listed terms and conditions from the search
- CAS Registry numbers are unique identifiers for chemical compounds – think of them as Social Security Numbers for chemicals. Knowing this number can help you search in other databases.

7. Break

10 minutes

8. Search for chemical properties in SciFinder

8.1. Background details

Let's search for the chemical properties of ferrocene in SciFinder.

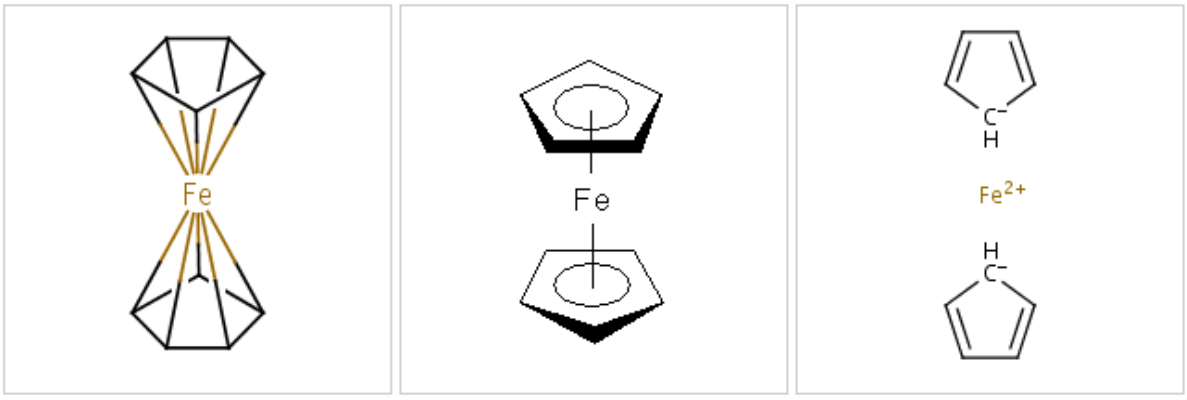
What is SciFinder?

- Database of scientific information in journal and patent literature from around the world, as well as reputable web sources
- References from more than 10,000 currently published journals and patents from more than 61 patent authorities
- Coverage from the present to the mid-1800s
- The world's largest collection of organic and inorganic substance information
- More details at http://www.cas.org/products/sfacad/index.html

Getting started with SciFinder

- First, register at http://software.chem.ucla.edu/scifind/UCBwebSFS.html
- Afterwards, log in at https://scifinder.cas.org/

While discovered in the last century, there is still no consistent way of drawing ferrocene. Here are some of ways that ferrocene has been drawn:



(a) (b) (c)

Source: Kirill. Drawing ferrocene. http://metallome.blogspot.com/2009/03/drawing-ferrocene.html (accessed 2010/9/5).

SciFinder has its own way of representing chemical structures – as outlined in the following table.

Table 4.1 *Overview of principal indexing issues for substances in REGISTRY*

Issue	Summary of general indexing	Example
σ-bonds (where both bond electrons are provided by one of the atoms in the bond)	Represented as a double bond between the atoms	Appendix A4.1.5
π-bonds	Represented as a single bond between all the participating atoms	Appendix A4.3.3
Stereoisomers	Represented by stereochemical descriptors in the name field and in the structure	Appendix A4.1.4
Isotopes	Hydrogen isotopes represented in the formula field; all isotopes represented in the name and structure fields	Appendix A4.1.3
Resonance	Special bond description ('normalized bond')	Appendix 5 and Section 5.2.3
Tautomerism	Individual valence bond structures of the tautomers are entered	Appendix 5 and Section 5.2.4
Alloys	When precise ratios of elements are known, the ratios are listed in the name and composition fields	Appendix A4.2.2
Salts	Generally indexed as two component substances with the acid and the base as separate components	Appendix A4.2.1
Mixtures, hydrates, host–guest complexes	Indexed as substances containing separate components	Appendix A4.2
Metal complexes	A variety of registrations depending on the nature of the complex	Appendix A4.3
Polymers	A variety of registrations but mainly as starting materials (separate components for the monomers) or as products (where the polymer has a precise structure repeating unit)	Appendix A4.4 and Section 6.10
Peptides/proteins	Peptides have sequence data; those with < 50 residues also have structure data	Appendix A4.4.4 and Section 6.9
Nucleic acids	Nucleic acids have sequence data; those with < 5 residues also have structure data	Appendix A4.4.5 and Section 6.9
Incompletely defined substances	A variety of registrations depending on the nature of the substance	Appendix A4.5.1
Minerals	Compositions, where known, are given in the name and composition fields; otherwise indexed by name only	Appendix A4.5.2
Natural oils, fats, etc.	Described by common or trade name, or by source in name and definition fields; in general they should be searched in CAPLUS by CA Index Name rather than by CAS Registry Number	Appendix A4.5.3

Source: Ridley, D. D., *Information retrieval: SciFinder*. 2nd ed.; Wiley: Hoboken, N.J., 2009.

8.2. Draw the structure for ferrocene (for a SciFinder search)

Ferrocene is a “pi-complex” because of the covalent pi-bonds between Cp and Fe.

According to the table above, how would you draw the structure for ferrocene when searching SciFinder?

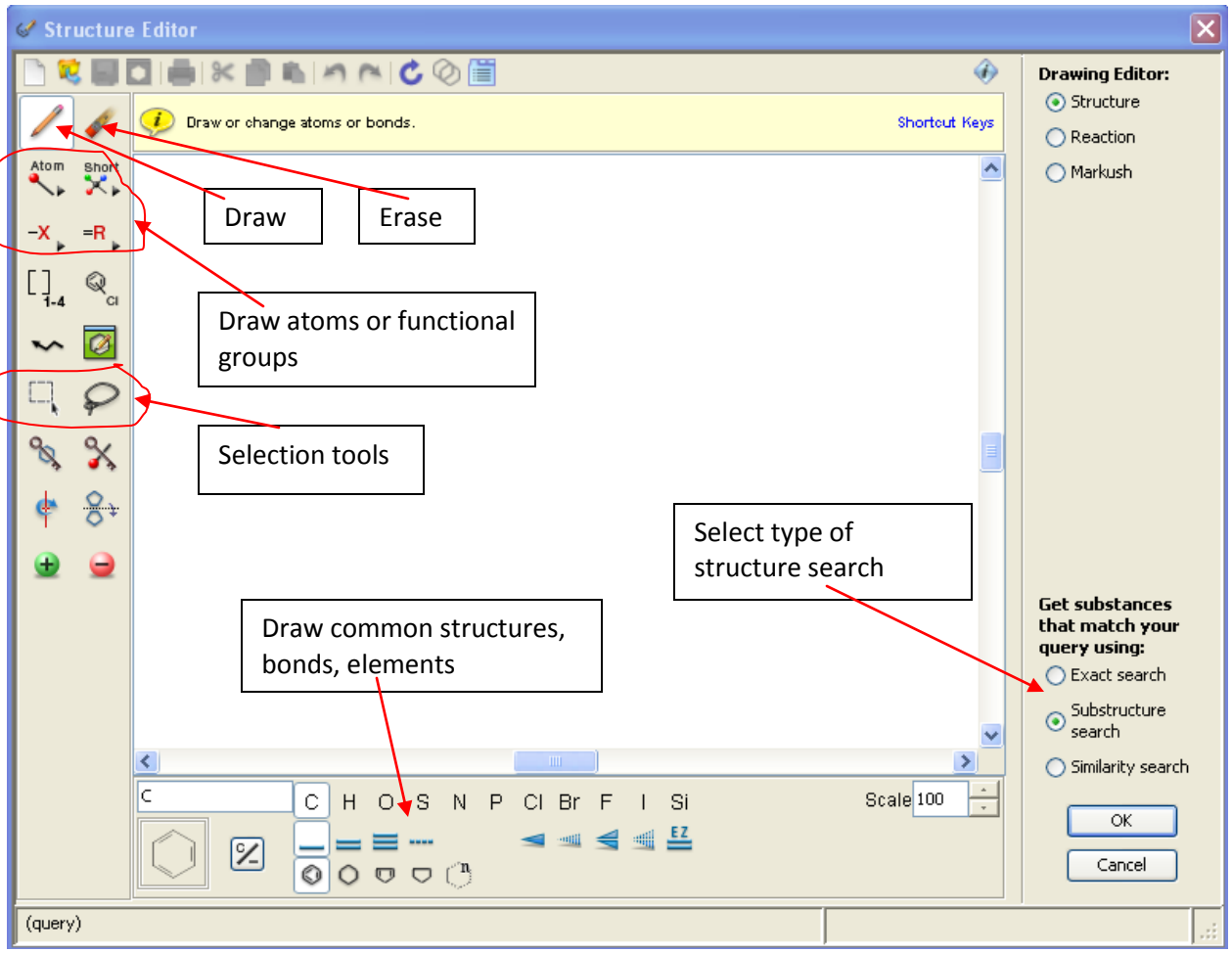
Remember: Ferrocene consists of Fe covalently bonded to 2 cyclopentadienyl rings ()


Please pause for class discussion.

8.3. Search SciFinder for ferrocene by chemical structure

1. Visit https://scifinder.cas.org/
2. Log in with your username and password.
3. Click *Accept* with the license agreement.
4. At the top, click 

5. In the chemical structure drawer, click *Click to Edit*.
6. Review the following diagram for the structure editor’s tools and functions.



7. Draw ferrocene according to the SciFinder convention.
   a. In the chemical structure drawer, click *cyclopentadiene* from the *common atoms, bonds, and structures menu* at the bottom.
   b. Draw 2 cyclopentadienes in the drawing area.
   c. (If you make a mistake) - Click on the select tool, make your selection, and then click delete. Alternatively, click the erase tool and make your deletion.
   d. Draw iron.
      i. Select 

and then select *Fe*.
      ii. Draw an iron atom between the cyclopentadienes.
   e. Draw the bonds between Fe and Cp according to SciFinder convention.
      i. Select an atom and then drag and drop to another atom.

8. At the bottom right hand corner of the structure editor, select *Exact search* to run an exact structure search, and then click OK.
    a. SciFinder warns you about overlaps detected. Click *Continue*.
    b. SciFinder warns you about exceeding standard valency. Click *Continue*.
9. Your structure is entered into the chemical structure search box.
10. FYI – take a look at the search options at the bottom of the screen.
11. Click the *Search* button.
12. How many substances do you find? _____

 Please pause for class discussion.

8.4. Post-activity discussion

- Using SciFinder
    - You need to register for SciFinder
    - SciFinder has a limited number of concurrent users
    - There are different ways of drawing chemical structures, therefore know the convention used in your database. Remember molecular formula searching may be easier sometimes.
- Even though an exact search was conducted, SciFinder retrieves ferrocene-containing complexes (i.e. compounds where ferrocene is a component).
    - In SciFinder, exact search results may include variations of the structure as you have drawn it, such as:
        - Charged compounds
        - Stereoisomers
        - Radicals or radical ions
        - Tautomers (including keto-enol)
        - Isotopes
        - Coordination compounds
        - Polymers, mixtures, and salts
- Click *Substance Detail* to see the following details:
    - CAS Registry Numbers for the compound and its components
    - Journal article references and other information resources (at the bottom of the record).
- Return to results by clicking on the breadcrumb trail at top.
    - 

- You can find commercial sources of substances by making your substance selections and clicking on the 

icon at top.

8.5. Find common chemicals quickly (by filtering search results by commercially availability)

In our search, we want to filter out the ferrocene-containing compounds in our search and just retrieve the ferrocene record.

We will try to do this by filtering our search results for commercially available compounds.

Why? What does this mean?

Ferrocene is a popular compound, and it is commercially available. (This means that you can order the compound from a vendor or supplier – and therefore, you do not have to synthesize the compound yourself.) By contrast, some of the ferrocene-containing compounds are obscure syntheses and are not commercially available.

If we filter by commercial availability, we might remove those obscure ferrocene-containing compounds from our search results.

1. In your ferrocene search results, go to the right-hand-side menu, and select the *Refine* tab.
2. Select *Commercial Availability* in order for SciFinder to filter out compounds that are commercially available and remove many of the obscure compounds.
3. Click the *Refine* button.
4. Review your results. Find the record that only contains ferrocene by itself.
5. Select *Substance Detail* to view the record for ferrocene.

8.6. Find chemical properties for ferrocene

1. In the ferrocene SciFinder record, look under *Spectra Properties*
2. View any one of the IR spectra by selecting *See spectrum*.
    a. What are the IR absorption peaks for ferrocene?

    _____

    _____

_____

_____

3. Go back to the substance record for ferrocene.
   a. What is the boiling point for ferrocene?

_____

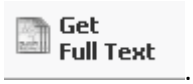
 Please pause for class discussion.

8.7. Post-activity discussion

- Filter results to find relevant records → Use the *Refine tool*
- Instead of commercial availability, you can use **Refine by "*Are a single component*"**
- Finding properties
  - You can check the references to see who made the measurement or determination. To do this, see the *Note* section.

8.8. DEMONSTRATION: Retrieve full-text journal articles from SciFinder

Let's examine the crystal structure for ferrocene.

1. In the ferrocene substance record, look under the *Structure-related Properties*.
2. For *Crystal Structure*, click the numbered reference. This opens the record for the journal article that reports ferrocene's crystal structure.
3. At the top of the record, click 

. This opens the journal article.
4. Click on *PDF* to see the publication-formatted version.
5. Skim the article.
6. Does this article give the crystal structure of ferrocene or a closely-related structure? (Alas, only a closely-related structure on page 2982 of the article).

9. Break

10 minutes

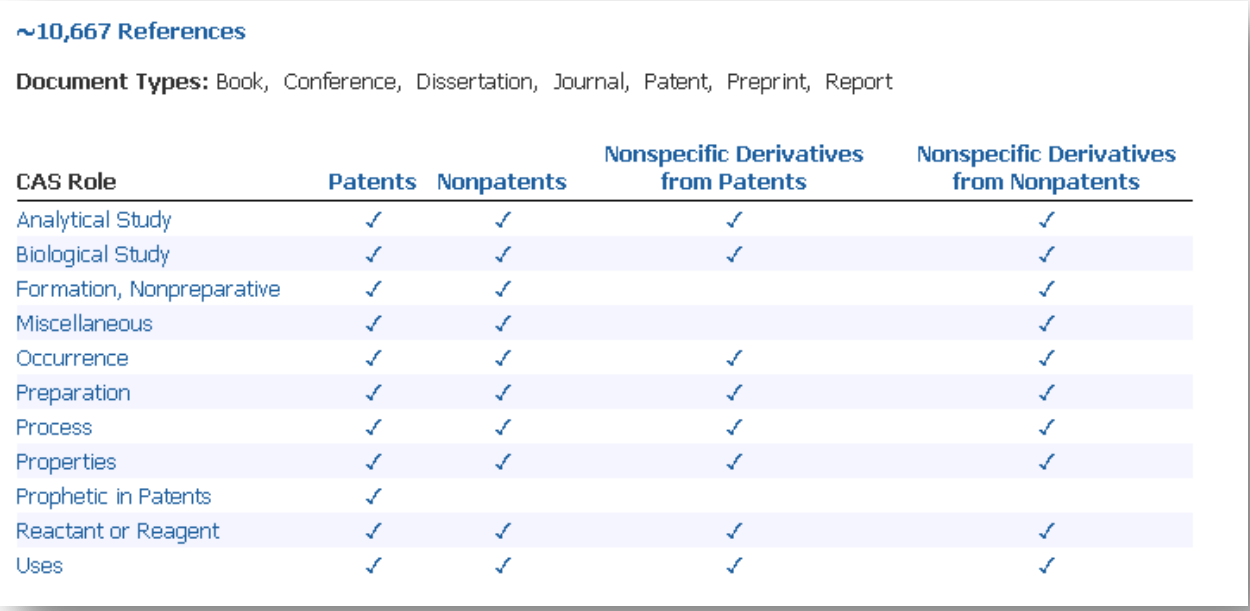
10. Find journal articles and publications about a compound

To see journal articles and other information about a compound:

- Go to the substance record
- Click on the link: ~ *# References*

There is a table that categorizes the articles and information by role.

- Click on a *checkmark* to see those materials.



~10,667 References

Document Types: Book, Conference, Dissertation, Journal, Patent, Preprint, Report

CAS Role	Patents	Nonpatents	Nonspecific Derivatives from Patents	Nonspecific Derivatives from Nonpatents
Analytical Study	✓	✓	✓	✓
Biological Study	✓	✓	✓	✓
Formation, Nonpreparative	✓	✓		✓
Miscellaneous	✓	✓		✓
Occurrence	✓	✓	✓	✓
Preparation	✓	✓	✓	✓
Process	✓	✓	✓	✓
Properties	✓	✓	✓	✓
Prophetic in Patents	✓			
Reactant or Reagent	✓	✓	✓	✓
Uses	✓	✓	✓	✓

10.1. Find one of the first articles on the preparation of ferrocene (using the SciFinder Refine function)

1. In the ferrocene SciFinder record, retrieve all references about ferrocene.
    a. Above the *Document Types* label, click on the link labeled ~ *# References*.
2. Ignore the limits, and click *Get*.
3. Let's work with a smaller set of results. Filter to journal articles that are published on the year Cyndi Lauper was born or earlier.
    a. Search Google to find the year she was born.
    b. In SciFinder, on the right-hand-side menu, select the *Refine* tab for the *Refine* function.
    c. Select *Publication Year*.

   d. Enter a search phrase to find all ferrocene articles published on the year Cyndi Lauper was born or earlier. How many articles are there? ___ ____

4. Above the search results, use the *Sort* menu to sort results by *Publication Year*.
5. What is the publication year of the oldest article in SciFinder that discusses ferrocene synthesis? _____

 Please pause for class discussion.

10.2. Write a reference citation in ACS style

1. In ACS style, write the reference citation for the oldest article in SciFinder that discusses ferrocene synthesis.
   a. Refer to section 4.2.2 on page 8 for tips.

 Please pause for class discussion.

10.3. Post-activity discussion (Finding first syntheses)

- SciFinder's *Refine* function filters your results and reveals more relevant materials
- SciFinder can help you identify one of the first articles published on a compound – but this is no guarantee that it describes the first syntheses.
- To find an article on the **first synthesis of a compound**:
  - Look for review articles or tertiary resources that describe the first synthesis. (Finding review articles are explained later.)
  - Sometimes the background/introduction of a current journal article may describe the first synthesis.

11. Learn about the history, current state, and the future of a research topic

11.1. Finding research articles for different time frames

The following table outlines where you can find literature about:

- the history of a research topic (past research, original work, classic works)
- the current state of a research arena, and
- the future (new directions for the research topic, evolving research work on the topic).

Time frame	Review articles	Books & the background section of journal articles	Primary journal article references	A journal article's future work section or conclusion
Historical works	Y	Y	Y	
Contemporary research	possible	possible	possible – references may point to contemporary studies	possible
Later developments or future work				Y

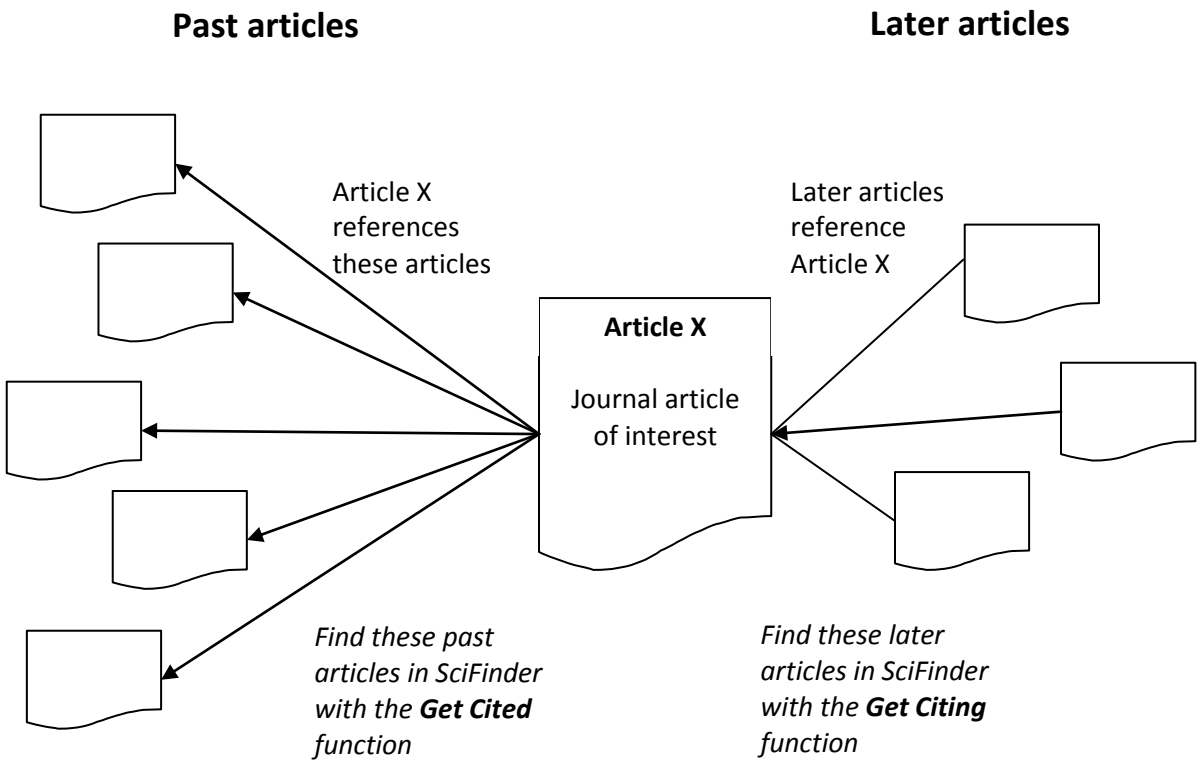
11.2. Cited reference searches help you learn about the "history" and the "future" of a research study

Suppose you find journal article X that discusses research on Compound Y or Topic Z.

Article X may discuss the historical perspective of a research topic and therefore cite articles from the past.

After Article X was published, researchers may have used Article X for newer research studies. These newer publications represent the later development of the original article X (i.e., the "future.")

The following diagram represents this relationship. At the bottom, cited reference searches are represented. Cited reference searches help you find what an article cites in a chronological context. In other words, **they help you find the "family tree" of a study**.



11.3. Run a cited reference search to find historical articles and later developments

We're going to examine the article:

Maroun, F.; Ozanam, F.; Magnussen, M.; Behm, R. J., The role of atomic ensembles in the reactivity of bimetallic electrocatalysts. *Science (Washington, DC, United States)* **2001,** *293* (5536), 1811-1814.

11.3.1. Quickly retrieve the SciFinder record for a journal article

1. At the top of SciFinder, select the *Explore References* icon.
2. On the left, select the *Journal* option.
3. Enter the journal article citation details for the above article.
4. Click the *Search* button.
5. In your search result, click on the article title to open the record and view the article's abstract.

11.3.2. Find articles cited (i.e., the "historical perspective")

1. In the journal article record, click on the *Get Cited* icon at top.
2. Using the *Sort by* menu above the results, sort the records by *Publication Year*.
3. What is the publication year of the oldest article cited? _____

11.3.3. Find later articles citing a study(i.e., "later developments" and "future work")

1. Go back to the SciFinder record for the original article (Maroun et al., 2001).
    a. Refer to the breadcrumb trail at top.
    b. Click on article title: "*The roles of atomic ensembles…*"
2. Now you're back in the record for the original article.
3. At the top, click the *Get Citing* icon.
4. How many journal articles reference Maroun et al. (2001)? _____
5. On the right-hand-side menu, select the *Analysis* tab. The analysis function groups the articles and runs statistics.
    a. Analyze by publication year. From the *drop-down menu*, select *Publication Year*.
6. How many research studies citing Maroun et al. (2001) were published in 2005?_____


Please pause for class discussion.

11.3.4. DEMONSTRATION: Use the Web of Science database for a cited reference search

1. Visit http://www.lib.berkeley.edu/CHEM/
2. Select *Web of Science*.
3. Select *Cited Reference Search*.
4. Enter journal article details and click search.
5. *Select* the citation, and click *Finish Search*.
6. Select the *UC-eLinks* button to view the full-text articles.

11.4. Post-activity discussion

- To learn about the history, current state, and the future of a research topic:
  - Read different types of resources
  - Run cited reference searches
  - Read a journal article carefully – particularly the background section and future work
- The SciFinder *Analysis* function categorizes reference articles and generates statistics on those groups.
- Cited reference searching helps you find the "family tree" of a study
  - In SciFinder use, the *Get Cited* and *Get Citing* tools
  - In the Web of Science database, use the *Cited Reference Search*
- UC-eLinks – Look for these buttons. They will retrieve full-text articles.

11.5. DEMONSTRATION: Find review articles in SciFinder for the history, background, overview, or interpretation of a topic

In SciFinder, after you run a search and have a set of journal articles, you can conduct an analysis by document type.

1. In your search results, select the *Analysis* tab.
2. In the drop-down menu, select *Document Type*.
3. Select *General Review*.

12. Recognize other ways of searching SciFinder (by research topic and reactions)

You can search SciFinder in other ways. Besides substance searching, you can search by:

- Chemical reactions
- Research topic

For instruction on these types of searches, visit http://www.cas.org/support/scifi/htguides.html

13. Break

10 minutes

14. Other inorganic chemistry information resources are available. Here's when you use them.

To connect to these resources from home or off-campus, find instructions by visiting http://www.lib.berkeley.edu/Help/connecting_off_campus.html

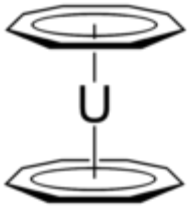
Resource	Description	Available through	Instruction
Cambridge Structural Database (CSD) System	The world repository of small molecule crystal structures. http://www.ccdc.cam.ac.uk/products/csd/	http://webcsd.ccdc.cam.ac.uk/	http://webcsd.ccdc.cam.ac.uk/help.php
Gmelin	Coverage back to the 1770's for inorganic and organometallic syntheses and property data.	Install the client program on your own computer. http://www.lib.berkeley.edu/CHEM/xfire.html#Access	http://www.info.crossfiredatabases.com/support/Gmelin%20_71_complete.pdf
Science of Synthesis	Online version of Houben-Weyl methods of molecular transformations containing approximately 2000 generally applicable synthetic methods in organometallic and heterocyclic chemistry covering 18,000 reactions with roughly 80,000 structures.	Please enable pop-ups in your web browser. http://www.thieme-chemistry.com/thieme-chemistry/sos/prod/user/index.html	http://www.science-of-synthesis.com/prod/pdf/gsm39.pdf
SciFinder	The world's largest collection of organic and inorganic substance information. A database of scientific information in journal and patent literature from around the world, as well as reputable web sources. References from more than 10,000 currently published journals and patents from more than 61 patent authorities. Coverage from present to the mid-1800s.	https://scifinder.cas.org/	http://www.cas.org/support/scifi/htguides.html
Web of Science	A citation database with multidisciplinary coverage of over 10,000 high-impact journals in the sciences, social sciences, and arts and humanities. It also includes international proceedings for over 120,000 conferences.	http://isiknowledge.com/wos	http://images.isiknowledge.com/WOK45/help/WOS/h_toc.html

14.1. DEMONSTRATION: Use Gmelin to find the average U-C bond distance for Uranocene

What is Gmelin?

- A database that specializes in inorganic compounds.
- It may serve as a backup to SciFinder for inorganic chemistry.

Here is uranocene, a coordination compound with 2 cyclooctatetraene ligands 



1. Start the *CrossFire Commander* client software.
2. Click *Select Database*.
3. Select *Gmelin*. Click *OK*.
4. On the left-hand-column menu, select the *Predefined Search Forms* tab.
5. Double click *Substance Identification Data*.
6. Enter the molecular formula for uranocene: $C_{16}H_{16}U$.
7. Click *OK*. The search phrase is entered into the search table.
8. Click *Start Search*.
9. Click *View* to open results.
10. Double click on the uranocene record.
11. The *Field Availability List* outlines the chemical properties, data, and information available. The following are of note for this class:
    a. Reaction
    b. History
    c. Reference

12. Let's find the average U-C (Go Bears!) bond length in uranocene. We'll look for its X-ray crystal structure.
    a. In the *Field Availability List*, click *CST* (Crystal Structure).
    b. In the references listed, click the *Full Text* button to open PDF journal articles that may give the bond lengths for uranocene.
    c. Review the second reference article. The average U-C length is 2.648 Å.

15. Use software to help you draw chemical structures and manage citations

- Molecule editor software
  - ChemDraw software lets you create, modify, and analyze representations of chemical structures. It is licensed by the College of Chemistry for its members.
  - To download and for support, please visit http://glab.cchem.berkeley.edu/glab/chemdraw.html

- Software for organizing and writing reference citations
  - RefWorks – bibliographic management software licensed for UCB faculty, staff, and students by the Library.
  - Get your free account via http://www.lib.berkeley.edu/CHEM/ref_end.html

16. Finding journal articles and books at the Chemistry library

The Chemistry & Chemical Engineering Library has **flow charts** that guide you through the process of retrieving journal articles and books.

- These flow charts are available for download at http://www.lib.berkeley.edu/CHEM/instruction/orientation/
- See page 6 and onwards.

If you are using an e-resource, remember to look for the **UC-eLinks** buttons that will help retrieve the full-text articles.

To decode a chemistry journal title abbreviation, search CASSI:

- http://cassi.cas.org/

17. Summary activity

Three new things that I learned today:

1.

2.

3.

Three things that I need to explore further:

1.

2.

3.

Notes

For further details, visit the:

- Library course page for Chemistry 108
  http://www.lib.berkeley.edu/CHEM/chem108.html
- Library website
  http://www.lib.berkeley.edu/CHEM/

Download this manual at:

- http://www.lib.berkeley.edu/CHEM/instruction/chem108