

ATTACH THIS COVER SHEET TO YOUR PRINTOUTS.

Chem 2219 FS2020
CLC Computer Problem Set
(37 pt total) **Due week of 10/26/20**

Name _____

Section _____

This assignment is to point out some online resources for information on organic compounds.

1. The *Journal of Chemical Education* is a publication targeted at high school and college chemistry instruction containing experiments, demos & theoretical articles on a wide variety of chemistry topics. The contents (1924-present) are searchable by topic, title, author, etc. and the article text and supplemental information is available via the MST library for free to current students.

Launch a browser and go to the *Journal of Chemical Education* at <http://pubs.acs.org/loi/jceda8>
Save as a browser bookmark for possible future use.

Use their online index search at the top of the screen to find a JChemEd article containing the term "hypochlorite oxidation". Click on "PDF" for the article titled "Oxidation of cyclohexanol to cyclohexanone by sodium hypochlorite"

Print out the first page only of the article and attach. **(5 pt)**

2. *SDBS* is an online database containing 34000+ free experimental FTIR, HNMR, CNMR, MS, Raman and ESR spectra, searchable by name, empirical formula, CAS#, MWt. It is also possible to search for spectra containing peaks at specific locations (ppm, cm-1, MS peak, etc. for help in identifying unknown experimental spectra)

Go to the *Integrated Spectral Database, SDBS*, site
http://sdb.sdb.aist.go.jp/sdb/cgi-bin/direct_frame_top.cgi

Save as a browser bookmark for possible future use.

Scroll to the bottom of the screen and click to agree with the disclaimer.

Find the structure, IR: liquid film and ¹H NMR spectra for 1-butanol. (Enter the name of the compound and click Search) Click on the HNMR spectrum. (Use the 90 MHz HNMR in CDCl₃ solvent)

Print out and attach. Be sure and also print the table with exact HNMR peak positions as well. **(6 pt)**

3. The *NIST Chemistry WebBook* is an online database of spectral and thermodynamic data for compounds. It is an alternative to the SDBS site.

Go to <https://webbook.nist.gov/chemistry/name-ser/> and enter cyclohexanone as the chemical species name. Find the IR spectrum (10% solution), print out and attach. **(5 pt)**

4. *Organic Synthesis* is a website and also a collection of hardcopy volumes in the library with synthetic procedures for organic compounds. Go to <http://www.orgsyn.org/Default.aspx>

Click on Search in the row near the top of the page.

Under *Search for the Following Text* on the next page, enter o-nitrobenzaldehyde and click Search. Find the one showing CrO₃, H₂SO₄ oxidation of 2-nitrotoluene and click PDF above the picture. Print the second page only in the resultant listing showing the summary of the procedure. **(5 pt)**

5. *SciFinder* is the online search engine for Chemical Abstracts, which contains all chemistry papers published in the world in any language. It also searches Medline, which contains medical information. It is searchable by topic, author, structure, formula, CAS#, journal, etc. It is updated weekly and is most effective at searching recent rather than older, (pre 1960s) articles. It is available to students for free and can be searched from your home if VPN is installed on your computer to identify you as a student.

Register for *SciFinder* at

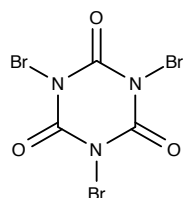
<https://origin-scifinder-cas-org.libproxy.mst.edu/registration/index.html?corpKey=4167C4E0-86F3-50AB-79CA-9F52F9C1CB36> .

There is a link to this registration on the chem 2219 (226) web page which is linked via the 2219 Canvas home page. The link is listed under General Organic Web Links.

Locate and start *SciFinder* via: Start → SciFinder Scholar Folder → SciFinder.

Click Accept. Click Continue.

Do a Chemical Structure search for the compound shown below by drawing it in the structure editor.



Click the CAS# above the structure that appears and scroll down the resulting page and note the last name listed under Other Names. Under CAS REFERENCE ROLES, click and select preparation non patents to bring up a list of articles. For the article in the European Journal of Organic Chemistry titled “Expedient Synthesis of Marine Natural Products Prepolycitrin A & B synthesis”, click *Other Sources*, then HTML from publisher. Click *Download PDF* to view the article in the resulting page. Scroll through the article to the Experimental Section and find the specific preparation instructions for the above compound.

Print out and attach that experimental page only of the article. (6 pt)

In SciFinder, for any article that appears from a search, the choice of *Quick View* and *Other Sources* is available below the title of the article. Even if the article is not in English, the *Quick View* will provide a short summary in English of what the article is about, the compounds used or conclusions reached.

If the library subscribes to the online journal, selecting *Other Sources* will connect you to the article via the *Web-based document resources* link that appears.

If the article is not available via electronic subscription, clicking on *Get it! @MST* under *Your organization's document resources* will connect you to the interlibrary request form so that the article can be ordered. This is free to students, but could take several days to arrive. You will receive an email with a link to the article when it arrives.

6. The *MST library* has numerous online journals. Go to the library homepage at <https://library.mst.edu> Click on *A-Z Electronic Journals* under the header at the top of the page.

Enter *Israel Journal of Chemistry* and click Search.

Click *Wiley Online Library Database Model 2020* on the resulting page.

(*The Academic Search Premier* link also works, but is more awkward to navigate).

Select 2012-volume 52, Issue 6. Find page 540 which is a review article on Indigo & Tyrian Purple, click PDF and attach the first page only. (5 pt)

Also draw the structure of Tyrian Purple given in the article. (5 pt)