

### ACS Style Guidelines for Citing Data

The examples below are suggested formats for citing data such as physical property data or spectra obtained from various types of resources. The ACS Style Guide provides a few examples for citing data but does not include examples of the wide variety of online sources that are available.

The purpose of the citation is to provide sufficient detail so that someone else can locate the data. Page numbers may not exist when citing online sources of data and therefore it may be necessary to indicate information like the CAS Registry Number or the entry name so that someone else can locate the exact information that was cited.

For more information consult the *ACS Style Guide: Effective Communication of Scientific Communication*, 3<sup>rd</sup> edition (Sciences and Technology Library Reference QD 8.5 A25 2006).

### Citation Examples for Citing Data

#### Web Sites

Web sites can be government sites, organization sites, course web sites or personal home pages. Some websites are considered databases and should be cited as a database. See the information on databases listed below. Databases include a reference number or other identifying information along with one or more search options.

#### General Features of Web Sites:

- accessible on the Internet
- no page numbers
- information cited is located at the URL provided – no additional searching is required

**Where to Find Citation Information:** Look at the About Us links, Contact Us links, Copyright link, copyright information at the bottom of the search screen, links with the word Citation or Cite. If a sample citation is provided it may not be in ACS Style.

**Basic Format:** Author, A. A. (if any). Title of Site. URL (accessed Month Day, Year), other identifying information (if any).

Web Site Examples	
Home page	Winter, M. WebElements: the periodic table on the WWW. <a href="http://www.webelements.com">http://www.webelements.com</a> (accessed Feb 1, 2013).
Specific section of a web site	Winter, M. Vanadium: the essentials. WebElements: the periodic table on the WWW. <a href="http://www.webelements.com/vanadium/">http://www.webelements.com/vanadium/</a> (accessed Feb 1, 2013).

## Databases

A database is a website that has a collection of information such as citations to journal articles, physical property data, or spectra. A database includes a search feature and individual records matching the query are retrieved. Most databases will include some unique identifier that will allow the user to retrieve that specific information again. Examples include: accession number, entry number, registry number, or chemical name.

### General Features of Databases:

- accessible on the Internet
- includes a search option
- individual entries identified by a unique number or an identifier such as a chemical name

**Where to Find Citation Information:** Look at the About Us links, copyright link, copyright information at the bottom of the search screen, links with the word Citation or Cite. If a sample citation is provided it may not be in ACS Style.

**Basic Format:** Author, A. A. (if any). *Title of Site*. Publisher: Place of Publication; Other identifying information such as the chemical name, registry number or entry number. URL (accessed Month Day, Year).

Database Examples	
Online database	Royal Society of Chemistry. <i>ChemSpider</i> . Caffeine, CSID=2424; <a href="http://www.chemspider.com/Chemical-Structure.2424.htm">http://www.chemspider.com/Chemical-Structure.2424.htm</a> (accessed June 15, 2011).
Online subscription database (URL includes proxy information from the library)	<i>Dictionary of Organic Compounds</i> . Taylor and Francis: Boca Raton, FL, 2013; RN 110-82-7; <a href="http://doc.chemnetbase.com">http://doc.chemnetbase.com</a> (accessed Feb 12, 2013).
SciFinder (spectra)	<i>SciFinder</i> ; Chemical Abstracts Service: Columbus, OH; carbon-13 NMR spectrum; spectrum ID CC-03-C_SPC-3734; RN 50-52-2; <a href="https://scifinder.cas.org">https://scifinder.cas.org</a> (accessed June 9, 2010).
SciFinder (calculated data)	<i>SciFinder</i> ; Chemical Abstracts Service: Columbus, OH; Density; RN 50-52-2; <a href="https://scifinder.cas.org">https://scifinder.cas.org</a> (accessed June 9, 2010); calculated using ACD/Labs software, version 11.01; ACD/Labs 1994-2013.
Spectral data from online database	National Institute of Advanced Industrial Science and Technology (AIST). <i>Spectral Database for Organic Compounds (SDBS)</i> ; mass spectrum; SDBS No.: 4778; RN 87-86-5; <a href="http://riodb01.ibase.aist.go.jp/sdbs/">http://riodb01.ibase.aist.go.jp/sdbs/</a> (accessed June 14, 2010).

Include home page URL for subscription sites without the proxy information.

The proxy information from the library can be removed from the URL. Example: proxy1.lib.umanitoba

## Exceptions

The example below appears to be more like a database but the Citation Guide on its website indicates that this source should be cited as a book.

NIST Chemistry WebBook	Stein, S. E. Infrared Spectra. In <i>NIST Chemistry WebBook</i> ; Linstrom, P. Mallard, W.G.; NIST Standard Reference Database Number 69; National Institute of Standards and Technology: Gaithersburg, MD, June 2005; RN 108-88-3; <a href="http://webbook.nist.gov">http://webbook.nist.gov</a> (accessed on Aug. 13, 2012).
------------------------	--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------

## Material Safety Data Sheets

**Basic Format:** *Title*; MSDS Number; [Online]; Manufacturing Company: Location of Company, Date. URL (accessed Month Day, Year).

Material Safety Data Sheets Examples	
Online MSDS	<i>Acetic Anhydride</i> ; MSDS No. A0338; [Online]; Mallinckrodt Baker: Phillipsburg, NJ., Feb 18, 2003. <a href="http://www.jtbaker.com/msds/englishhtml/a0338.htm">http://www.jtbaker.com/msds/englishhtml/a0338.htm</a> (accessed Dec 12, 2012).
MSDS obtained from a database source such as CCOHS	<i>Titanium Dioxide</i> ; MSDS No. T3627; Mallinckrodt Baker: Phillipsburg, NJ, November 12, 2003. Available from Canadian Centre for Occupational Health and Safety. <a href="http://ccinfoweb2.ccohs.ca/msds/Action.lasso?-database=msds&amp;-layout=Display&amp;-response=detail.html&amp;-op=eq&amp;MSDS+RECORD+NUMBER=3767394&amp;-search">http://ccinfoweb2.ccohs.ca/msds/Action.lasso?-database=msds&amp;-layout=Display&amp;-response=detail.html&amp;-op=eq&amp;MSDS+RECORD+NUMBER=3767394&amp;-search</a> (accessed Apr 14, 2005).

## Online Books

An online book generally corresponds to the printed version. Cite books like print-based books but add [Online] after the title. Page numbers are usually available. Some online books also have interactive tables that do not have page numbers. Cite the table and indicate the substance or other identifying name in the table instead of the page number.

### General Features of Online Books

- page numbers available
- table of contents and chapters usually available
- sometimes have interactive tables without page numbers

**Where to Find Citation Information:** Some online books will provide a basic citation. Look for the words Citation or something like Cite this Book. These citations will not necessarily be in ACS style but will give you clues as to what information to cite. Also check the Front Matter section, Preface or book cover.

### Basic Format for Online Books with Editors:

Author 1; Author 2; Author 3; etc. Chapter Title. In *Book Title* [Online]; Editor 1, Editor, etc. Eds.; Series Information (if any); Publisher: Place of Publication, Year; Volume Number, Pagination or Name of Compound or other identifying information; URL (accessed Month Day, Year).

Online Book Examples	
Interactive Table from an Online Book with Editor (example 1)	Physical Constants of Chemical Substances. In <i>Dictionary of Substances and Their Effects</i> . 3 <sup>rd</sup> Electronic Edition. [Online]; Gangolli, S. Ed.; Royal Society of Chemistry: Cambridge, 2005; RN 67-64-1; <a href="http://www.knovel.com/web/portal/basic_search/display?_EXT_KNOVEL_DISPLAY_bookid=527">http://www.knovel.com/web/portal/basic_search/display?_EXT_KNOVEL_DISPLAY_bookid=527</a> (accessed Jan 30, 2013).
Interactive Table from an Online Book with Editor (example 2)	Physical Constants of Organic Compounds. In <i>CRC Handbook of Chemistry and Physics</i> . 93rd ed.; [Online]; Haynes, W. M., Ed.; CRC Press: Boca Raton, FL, 2013; RN 110-82-7; <a href="http://www.hbcnetbase.com">http://www.hbcnetbase.com</a> (accessed Feb 1, 2013).

The proxy information from the library can be removed from the URL. Example: .proxy2.lib.umanitoba.

Use the home page URL only without the proxy information.

## Print Books

**Where to Find Citation Information:** Check the title page and copyright information page.

Print Books Examples	
Edited Book	<i>The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals</i> , 12th ed.; Budavari, S.; O'Neal, M.J.; Smith, A.; Heckelman, P. E.; Kinneary, J. F., Eds.; Merck & Co.: Whitehouse Station, NJ, 1996; entry 4857.
Edited Book	<i>CRC Handbook of Chemistry and Physics</i> , 89th ed.; Lide, D.R., Ed.; CRC Press: Boca Raton, FL, 2008; Section 3, No. 339.
Data set compilation	<i>The Sadtler Spectra: 300 MHz Proton NMR Standards</i> ; Bio-Rad, Sadtler Div.: Philadelphia, PA, 1994; no. 7640 (1-Chloropentane).

The above examples were developed based on the following guidelines from the ACS Style Guide:

“References to data should include the data entry number or other identifying information at the end of the citation. The date of access can also be included if the database is updated frequently. If the data retrieved are calculated data, also cite the software used for the calculation (for example, ACD/Labs).” (ACS Style Guide, p. 324)

“Data sets are compilations of data, such as spectra or property tables. These data sets are often published serially as loose-leaf services, but the content is not always organized in chapters as in other serial publications. The citation of a serial data set should contain the title of the data set, the publisher, the place of publication, the date of the volume, the data entry number (as opposed to the data value), and the name of the figure or other identifying information. The page number can be included in the citation if page numbers are used in the index of the data set.” (ACS Style Guide, p. 314)

“For material other than books and journals, sufficient information must be provided so that the source can be identified and located.” (ACS Style Guide, p. 290).

## **Other Resources for Citing Books, Journals and Other References**

The following resources provide examples of citing other types of references using ACS Style.

[ACS Style Guide – Chapter 14 References](#)

[ACS Citation Style - Concordia University Libraries](#)

[ACS Style Guidelines – UW- Madison Libraries](#)

[Cite Source, Trinity College Library](#)

[Quick Guide to ACS Style – Penn State University Libraries](#)