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Finding Physical Properties of Chemicals: A Practical Guide for Scientists, Engineers, and Librarians

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IMPORTANT NOTE: The web site ChemFinder reviewed in the original article has changed its name to ChemBioFinder and has eliminated physical property data, excepting in CambridgeSoft subscription databases. All references to ChemFinder have been removed from this updated version.

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SUMMARY. Free Internet resources that provide a significant amount of physical property information are critically reviewed. These free Web sites can not totally replace classic print sources and online subscription databases. However, a number of these Web sites provide extensive and reliable property information, especially for substances that are used in commerce or have seen significant research interest. This guide will be of particular value to those with occasional needs for physical properties or working without the benefit of access to a major research library and its subscription-based electronic resources.

KEYWORDS. Physical properties, chemical compounds, Internet resources, World Wide Web guides, critical review, chemical information

INTRODUCTION & METHODOLOGY

This article describes and evaluates the various Internet resources that provide significant physical property information and are available on the Web for free. Registration may be required, but no access fee is charged. Particular attention was paid to sites providing data for a large number of substances or a large number of properties, or both. This review focuses on chemicals, i.e. individual substances. Excluded were sources specific to toxicological and environmental information[1-6], biomolecules[7-9] such as enzymes, spectra[10-12], atomic data[13], and property estimation software[14-15]. Each of those areas would be a major guide unto itself. Small, specialized engineering materials Web sites were also excluded, though some of the larger comprehensive sites are reviewed, especially in the polymer area. Three recently published reviews provide a more in-depth look at materials science resources.[16-18]

A careful survey of existing science-oriented Web guides, metasearch sites, and Web directories was made to develop as complete a list of sites as possible. Included in this were academic Web guides at Trinity University, Univ. of Chicago, Vanderbilt University, University at Buffalo, and Indiana University. Property information listed in standard directory guides were reviewed from *About* (*http://www.miningco.com*), *Invisible Web* [no longer available], *Open Directory Project* (*http://dmoz.org/*), and the Univ. of Wisconsin *Internet Scout Project* (*http://scout.cs.wisc.edu/*). Personal bookmarks gathered from many years in chemical information work and listserv postings were also checked.

THE IDEAL WORLD

In an ideal world, all scientific libraries would have at their immediate disposal the many fine printed reference works and subscriptions to the major electronic databases covering physical properties. Given

that many of the printed sources are very old and out-of-print, these perfect-world libraries would also have been in existence for decades and never had any budget difficulties! A list of their holdings would include: [Key: (p=print, e=electronic)]

Scifinder® or SciFinder® Scholar [Chemical Abstracts Service] (e)
Beilstein Handbook (p) or CrossFire™ Beilstein [MDL Information Systems] (e)
Gmelin Handbook (p) or CrossFire™ Gmelin [MDL Information Systems] (e)
Landolt-Börnstein Numerical Data & Functional Relationships [Springer-Verlag] (p,e)
International Critical Tables [U.S. National Research Council] (p)
The full spread of STN® International Databases (e)
Standard Reference Data Program Publications [U.S. Nat. Inst. of Standards & Technology (NIST)] (p,e)
Design Institute for Physical Properties (**DIPPR**)® Publications (p,e)
Thermodynamics Research Center (TRC) publications [Texas A&M Univ.] (p,e)
Center for Information and Numerical Data Analysis and Synthesis (CINDAS) publications [Purdue Univ.] (p,e)
Handbook of Environmental Data on Organic Chemicals [Wiley] (p)
Dictionary of Organic Compounds and other Chapman Hall/CRC dictionaries (p,e)
Journal of Chemical and Engineering Data [American Chemical Society] (p,e)
Journal of Physical and Chemical Reference Data [Amer. Inst. of Physics/NIST] (p,e)

There are many reviews of the major print and electronic reference sources in individual articles and chemical information resource textbooks.[19-24]

I. STARTING POINTS

A) Manufacturer/Supplier Web Sites

Most chemical companies and laboratory chemical supply firms provide at least basic data for the products they manufacture or sell on their Web site. It is common to find material safety data sheets (MSDS) and technical bulletins online. For example, technical bulletins will often give extensive electrical properties for polymers used in electronics applications.

This is an obvious starting point for trademarked materials, but is also useful for basic, large volume chemicals. Once a manufacturer or supplier has been identified via standard sources, any good Internet search engine should readily provide a link to the company Web site. Chemical company URL's can be identified via Web directories such as:

- *ChemIndustry.Com* (*http://www.chemindustry.com/*)
- *MSDS Provider* (*http://www.msdsprovider.com/Site/msdsprovider.nsf/search*)
- *ChemExper Chemical Directory* (*http://www.chemexper.com/*)

The last two Web sites provide links to the supplier's Web site, at times directly to the full-text of the MSDS. *ChemExper* is discussed more fully in the Web site survey section of this article. Where the company name is known, use of a general search engine such as *Google* (*www.google.com*) can often identify the needed company home page just as quickly.

Four examples of the thousands of commercial product information Web pages are:

- DuPont Elastomers *http://www.dupontelastomers.com/Header/index.asp*
- Occidental Chemical *http://www.oxychem.com/products/detailed-product.html*
- Acros Organics *http://www.acros.be/*
- Sigma-Aldrich Companies *http://www.sigmaaldrich.com/*
- Most corporate sites require a simple registration to view their technical product literature. However, there is seldom a fee for registration or much risk of triggering unwanted junk mail.

B) MSDS Compilations

There are several excellent Web guides and compilations of material safety data sheets (MSDS). Keep in mind that MSDS, especially from laboratory supply firms, give only the basic properties, and

many times a number of these are left blank. Finding viscosity or thermal expansion, for example, is unlikely, unless that property is of particular importance in the substance's handling or use. A few of the best MSDS sites are listed below in Table 1.

TABLE 1: Select MSDS Compilations on the Internet

NAME	# of MSDS	URL
Cornell University	250,000	decomissioned as of March 15, 2007
Vermont SIRI (mirror site)	180,000	http://siri.org/msds/
Interactive Learning Paradigms Where to Find MSDS.	Web Guide	http://www.ilpi.com/msds/index.html
MSDS-Search	Web Guide	http://www.msdssearch.com/

II. SURVEY OF PHYSICAL PROPERTY WEB SITES

When searching for physical properties, one quickly learns that well-known properties for common chemicals can be readily found in almost any source covering physical properties: basic handbooks, encyclopedias, chemical catalogs, and Internet sites. However, most patrons seeking the assistance of an information professional are more likely than not to have an uncommon chemical or an unusual property or both.

The resources discussed in the rest of this paper can not take the place of having access to the major reference books and subscription resources such as Landolt-Börnstein, STN International numerical databases, or publications from the government-sponsored thermodynamic data projects like Texas A&M University's TRC. Nor is there any substitute for a full retrospective search of the primary literature via Gmelin, Beilstein, and Chemical Abstracts. These points are clearly demonstrated by the comparison of coverage of the major free Web sites versus the subscription CrossFire Beilstein and Gmelin products available from MDL Information Systems. This comparison is presented after the discussion of the five largest property Web sites. However, there is a growing body of usable and generally reliable data available for free on the Web.

All the Web sites evaluated in this article are summarized in Tables 2, 4, 5, and 6. Column 2 (# of compounds) reflects the approximate number of compounds covered, which changes as the site is updated. Column 3 (max. # of properties) is the approximate maximum number of properties potentially available directly from the Web site. Some Web sites contain links to additional properties on other Web sites. The "Searchable by" columns reflect the ways in which the data can be searched. In order:

- Name - Chemical/common name
- CAS RN - Chemical Abstracts Service Registry Number
- MF - Molecular formula
- MW - Molecular weight
- Prop Values - Range-searchable property values.
- Substruct. - Substructure searchable

A. *The Large Players: Recommended First Stops on the Web*

Four Web sites have been identified that each cover more than 20,000 substances: *NIST Chemistry WebBook, ChemExper Chemical Directory, Matweb,* and the *Physical Properties Database (PHYSPROP)* developed by the Syracuse Research Corp. The first three on this list are particularly important to consult in almost any physical property search.

TABLE 2 - Evaluated Web Sites: Large Players and General Sites

			Searchable by:							
Web Site Name	**# of compds**	**Max. # props**	Name	CAS RN	MF	MW	Prop Values	Substruct.	**Type**	**Sponsoring Organization**
The Large Players										
ChemExper Chemical Directory	70,000	4	x	x	x	x	x	x	Metasearch	ChemExper
Matweb	25,412	75	x				x		Database	Automation Creations
NIST Chemistry WebBook	40,000	45	x	x	x	x	x	x	Database	U.S. NIST
Physical Properties Database (PHYSPROP)	25,250	8		x					Database	Syracuse Research Corp.
General, Smaller Scale Web Sites										
Estimation Program Interface (EOI) Suite		14		x					Estimator	U.S. EPA/Syracuse Research Corp.
Hazardous Chemical Database	3,995	10	x	x	x				Database	Univ. of Akron
Hazardous Substances Data Bank	4,500	30	x	x	x	x		x	Database	Nat. Lib. Of Med.
International Chem. Safety Cards	675	10	x	x					Table	NIOSH/WHO/ILO
NTP Chemical Health & Safety Data	2,000	28	x	x	x				Database	U.S. NIEHS - Natl. Toxicology Program
Organic Compounds Database	2,483	5	x		x	x	x		Database	Colby College

1) ChemBioFinder ***[no longer provides property information. This section has been deleted.]***

2) *NIST Chemistry WebBook* (*http://webbook.nist.gov/chemistry/*)

As befits the National Institute of Standards and Technology (formerly the National Bureau of Standards), the data quality and usability of this Web site is first rate. Up to forty-five thermochemical, thermophysical, and ion energetics critically reviewed properties are available for over 40,000 compounds. The data has been compiled from the NIST Standard Reference Data Program and outside contributors. The source of all data and, frequently, the method are carefully documented. Comments provide additional information such as the uncertainty of the measurement. Most of the data is in tabular form, but some can be displayed as X-Y plots. In addition, mass, IR, and UV/Visible spectra are provided in graphical form.

The database is predominantly organic with a few small inorganic compounds. A full spectrum of search options exists including names, CAS registry numbers, property ranges, and substructure. Author searching permits one to check what literature references have been used in compiling the database. For each retrieved substance, basic information including molecular formula, synonyms, and structure are provided along with links to the various categories of properties.

3) *ChemExper Chemical Directory (http://www.chemexper.com/)*

This site provides a metasearch of over 70,000 chemicals from more than twenty supplier catalogs. The directory can be searched by registry number, molecular formula, chemical names, physical and chemical characteristics, and substructure. Links are provided to the supplier's Web site and to 16,000 MSDS, mostly from Acros. Only the basic properties are directly provided: density, m.p., b.p., and flash point. However, links to the full-text of the MSDS will usually provide some additional properties.

The ChemExper company, based in Belgium, encourages both commercial suppliers and academic laboratories to submit product information directly into the database. Though all organizations submitting data are registered, clearly the property data is not critically reviewed and should be used with caution. However, this directory provides a quick way to determine basic properties and laboratory-scale suppliers for a wide range of substances available commercially.

4) *Matweb (http://www.matweb.com/index.aspx)*

Although this article does not attempt to cover the dozens of small, specialized engineering materials resources, the *Matweb* site is particularly comprehensive, covering over 25,400 materials. Included are polymers, metals, alloys, superalloys, ceramics, glass, fibers, composites, semiconductors and aerogels. Up to seventy-five properties are available for each material. Searching can be done by material type, trade name, specification number, manufacturer, up to three different property ranges, and alloy composition ranges. Automation Creations Inc., designer and maintainer of this site, also encourages submission of additional materials and data from companies. For a small subscription fee, additional features and search options are available.

5) *Physical Properties Database - PHYSPROP*
(http://www.syrres.com/what-we-do/databaseforms.aspx?id=386)

The Syracuse Research Corporation has developed a series of environmental chemistry databases, supported partially by the United States Environmental Protection Agency (EPA), Procter and Gamble, and DuPont. *PHYSPROP* contains chemical structures, names, and physical properties for over 25,250 chemicals. Some of the values are estimated rather than experimental. Up to eight physical properties are provided: m.p., b.p., water solubility, octanol-water partition coefficient, vapor pressure, pKa (acidity), Henry's law constant, and OH rate constant in the atmosphere.

This free demo database can only be searched by CAS registry number. Full literature references are not given. Only the authors and year of publication are provided. Of course, with a little information detective work, the full reference could be identified. The free database also does not have the substructure searching capabilities that are available with the ISIS/Base (MDL Information Systems, Inc.) or the Accord for Access (Synopsys Scientific Systems, Ltd.) commercial versions of *PHYSPROP*. A fuller review of environmental Web sources has been provided by Stoss[6].

B) *Comparison of the Large Free Sites Vs. a Subscription Source*

A study was made of the number of properties covered by the large Web sites described in the last section as compared to the Web versions of the classic Beilstein Handbook (organic chemicals) or Gmelin Handbook (inorganic chemicals). The *Matweb* site was excluded from this comparison since it deals mostly with materials, instead of individual chemical substances.

The Beilstein and Gmelin handbooks have been premier sources of physical property information for well over a century. Within the past decade, this information has been made available on the Web on a subscription basis by MDL Information Systems' CrossFire search system.

Ten chemicals were searched against *NIST Chem WebBook, ChemExper, PHYSPROP*, and then Beilstein or Gmelin as appropriate. The chemicals were purposefully chosen to range from the very common (phenol) to a specialized research chemical (1-(2-pyridinyl)piperazine). The results are given in Table 3. The number of references in CAS' CAPlus database shown in the third column provide a good indication of how common the substance is. Though limited in scope, this comparison shows the value and limits of free Web sources versus a high quality, but admittedly expensive, online database.

The number of unique properties, not including spectra, was carefully determined for each compound at each Web site. This data shows that the *NIST Chem WebBook* is the most comprehensive free Web site (184 total property values). The other three sites range from fifty-nine values for *ChemExper* to sixty-eight for *PHYSPROP*. What really stands out are the properties available from the CrossFire products, 459 properties which is 2.5 times more than the best free site, *Chem WebBook*. The free Web can not match fee services in this area.

TABLE 3: Comparison of the Free Web Vs. a Subscription Service

Chemical	CAS Registry Number	CA Hits	*NIST Chem WebBook*	*ChemExper* (incl. MSDS)	*PHYSPROP*	Beilstein/Gmelin Crossfire
Phenol	108-95-2	51,781	25	8	8	70
Aniline	62-53-3	34,059	28	9	8	68
Cyclohexane	110-82-7	25,539	35	8	7	72
Monochlorobenzene	108-90-7	14,255	26	10	7	69
Sodium Acetate	127-09-3	9,262	7	2	5	31
Phosphine	7803-51-2	6,275	15	0	7	43
Ciprofloxacin	93107-08-5 85721-33-1	6,155	0	0	5	12
Ethanethiol	75-08-1	4,152	26	10	8	47
Benzotrifluoride	98-08-8	1,023	22	7	7	40
1-(2-pyridinyl)piperazine	34803-66-2	545	0	5	6	7
Total Properties not counting spectra			**184**	**59**	**68**	**459**

C. General, Smaller Scale Web Sites

1) *Estimation Program Interface (EPI) Suite (http://www.epa.gov/oppt/exposure/pubs/episuite.htm)*

This handy software was developed by the Syracuse Research Institute under U.S. EPA contract. It is reviewed here because, unlike most property estimation programs, it is available as freeware. By entering a single SMILES notation as the search key, results from ten separate programs are displayed:

Aquatic toxicity (LD50, LC50)	Henry's law constant
Aqueous hydrolysis rates	M.P, B.P., and vapor pressure
Atmospheric oxidation rates	Octanol-water partition coefficient
Bioconcentration factor (BCF)	Soil sorption coefficient (Koc)
Biodegradation probability	Water solubility

The program contains a SMILES notation database searchable by CAS registry numbers. By entering a registry number, the SMILES notation is automatically retrieved and entered into the search box.

2) *Hazardous Chemical Database (http://ull.chemistry.uakron.edu/erd/)*

The University of Akron maintains a database that gives the set of physical properties commonly found on MSDS for about 4,000 compounds. Though there is little information that could not be found in other sources, it does present the data concisely and clearly.

3) *Hazardous Substances Data Bank (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB)*

This database from the National Library of Medicine should be familiar to anyone working in the environmental chemistry and toxicology fields. In addition to a very fine review of all environmental and health aspects of over 4,500 chemicals, the physical property section of these lengthy records provides up to ten of the more common properties. Unlike many free resources, the property values are critically reviewed and documented with the full literature reference.

4) *International Chemical Safety Cards (http://www.cdc.gov/niosh/ipcs/nicstart.html)*

These safety cards are two-page summaries of basic hazard information for 675 of the most common chemicals in international commerce. The physical property section provides the typical eight to ten

properties found on most MSDS. The World Health Organization, Commission of the European Communities, International Labour Organization, and NIOSH jointly sponsor this program.

5) *NTP Chemical Health & Safety Data (*http://ntp.niehs.nih.gov/index.cfm?objectid=03610FA5-C828-304B-FE31F1182E8F764C)

NTP no longer maintains this data and refers users to:

- National Institute for Occupational Safety and Health's ***"NIOSH Pocket Guide to Chemical Hazards"*** (http://www.cdc.gov/niosh/npg/npg.html)
- NIOSH also provides links to other sources via (http://www.cdc.gov/niosh/database.html)
- National Library of Medicine's ChemIDplus (http://chem.sis.nlm.nih.gov/chemidplus/)

6) *Organic Compounds Database (http://www.colby.edu/chemistry/cmp/cmp.html)*

Maintained at Colby College, this site features a database of 2,483 compounds compiled by Harry M. Bell of Virginia Tech. Though only a few common properties are provided, the search screen allows the selection of a wide variety of parameters including property values, element counts, and the presence or absence of certain broad structural entities such as amines or hydroxyl groups. Unfortunately, retrieval sets are limited to twenty compounds, though the search engine does report the total number of hit compounds.

D. Sites Focusing on Specific Types of Material

TABLE 4 - Evaluated Web Sites: Specific Types of Material

Specific Types of Material Web Site Name	**# of compds**	**Max. # props**	Name	CAS RN	MF	MW	Prop Values	Substruct.	**Type**	**Sponsoring Organization**
ARS Pesticide Properties Database	324	16	x						Table	USDA Agricultural Research Service
Critical Properties of Gases	700	3	x		x	x			Table	Flexware
Fuel Property Database	27	29	x				x		Database	DOE - Office of Transportation Technol.
NIST Ceramics WebBook	265 families	40	x						Database	U.S. NIST
Plastics Additives Database	9,500	Varies	x		x				Database	Specialchem
Plastics Technology Materials Database	13,200 grades	Varies	x		x		x		Database	Plastics Technology Magazine
Solv-DB	224	44	x	x	x	x	x		Database	Nat. Center for Manufacturing Sciences

1) *ARS Pesticide Properties Database (http://www.ars.usda.gov/services/docs.htm?docid=14199)*

Developed by the U.S. Department of Agriculture's Agricultural Research Service (ARS), this database is a compendium of chemical and physical properties of 334 widely used pesticides. Information included in the database focuses on sixteen of the most important properties that affect pesticide transport and degradation characteristics. References are provided for all data. Property values have been rechecked with the manufacturers for accuracy. Access is by pesticide name only.

2) *Critical Properties of Gases (http://www.flexwareinc.com/gasprop.htm)*

This simple, but useful table from Flexware provides mole weight, critical pressure and critical temperatures for about 700 gases. Inorganics and organics are both included.

3) Advanced*Fuel Properties Database (http://www.nrel.gov/vehiclesandfuels/fuels_database.html)*

This database that provides key data on about 33 advanced compression ignition fuels, such as biodiesel and synthetic diesel. Created by the U.S. Department of Energy (DOE) Office of Transportation Technology, included is information on various physical, chemical, operational, environmental, safety, and health properties. The source and standard test methods used are also given.

4) *NIST Ceramics WebBook (http://www.ceramics.nist.gov/webbook/evaluate.htm)*

The *NIST* (U.S. National Institute of Standards and Technology) *Ceramics WebBook* consists of two searchable databases, *High-Temperature Superconductors (WebHTS)* and *Structural Ceramics (WebSCD)*, and one browsable collection of property data summaries (*WebPDS*) for six categories of ceramics. As befits an NIST effort, the data source and quality are carefully reviewed and documented. Once a particular material has been retrieved, the format of the display is very similar to the better-known *NIST Chemistry WebBook*. Hyperlinked property categories take you to the exact point on the Web page displaying the information desired.

The Superconductor database provides evaluated thermal, mechanical, and superconducting properties for oxide superconductors. Materials are searchable by chemical family, informal name, structure type, and desired property. Authors' last name, publication source, and publication year are also searchable. The tables for a given property can be quite lengthy since they show values based on the mass fractions of the various component oxides.

The Structural database provides evaluated data for a wide range of structural, engineering, and fine ceramics. The search input form and display features are identical to the Superconductor database.

5) *Plastics Additives Database (http://www.specialchem.com/customers/demo/formSearchProduct_demo.asp)*

Specialchem operates a set of free information services to link users and suppliers of plastic additives. A 9,500 product database from about 260 suppliers can be searched by additive function, base polymer, trade name, supplier, and keywords. The search can be limited to additives approved for food contact. Technical articles, datasheets, links to supplier Web sites, and Web forms for requesting quotations, technical data, or samples are available. Free registration is required to display much of the information.

6) *Plastics Technology Materials Database (http://www.plasticstechnology.com/dp/materials/)*

Plastics Technology Magazine provides information on over 13,190 grades of plastics. They are searchable by about sixty properties, supplier name, resin family, descriptive terms like color, and price ranges. As expected, properties related to processing and use of plastics such as cure time, melt viscosity, impact strength, and flammability are emphasized. The search system is quick and easy to navigate. Particularly useful is the ability to display the results in a user-customized table format. What appears to be an older version of the same database is available from Bill Communications under the name *Plaspec Materials Selection Database* (*http://www.plaspec.com/index.html*), a web site that may be useful for discontinued products.

7) Solv-DB (http://solvdb.ncms.org/solvdb.htm)

Sponsored by the National Center for Manufacturing Sciences (NCMS), at least 224 solvents can be searched by eight different parameters including solvent name, CAS registry number, molecular formula, and chemical category. Nine different properties are range searchable including flash point, vapor pressure, density, and surface tension. Up to thirty-three more properties can be displayed for each solvent. Results can be sorted by solvent name or any of the nine range-searchable properties. Extensive information is provided for each solvent with display of health, safety, regulatory, and environmental fate data.

E. Sites Focusing on Specific Properties

TABLE 5 - Evaluated Web Sites: Specific Properties

Specific Properties Web Site Name	# of compds	Max. # props	Name	CAS RN	MF	MW	Prop Values	Substruct.	Type	Sponsoring Organization
Acoustic Material Property Tables	470	6	x						Table	Specialty Information Associates
ATHAS Data Bank of Thermal Properties	200	8	x						Table	Univ. of Tenn/Oak Ridge Natl Lab.
Dielectric Constant Reference Guide	1,500	1	x						Table	ASI Instruments
Pesticide Fact Sheets - New Active Ingredients	42	16	x						Table	U.S. EPA
Phase Diagrams Web	900		x						Table	George Tech Joint Student Chapter of ASM/TMS

1) *Acoustic Material Property Tables (http://www.ultrasonic.com/tables/index.htm)*
Specialty Information Associates maintains this simple, but effective, set of tables in MS Excel format providing six different acoustic properties of materials. Solids, plastics, rubbers, liquids, and gases are all covered. A table of longitudinal and shear piezoelectric information is also provided.

2) *ATHAS Data Bank of Thermal Properties (http://athas.prz.rzeszow.pl/Default.aspx?op=db)*
The Advanced Thermal Analysis Laboratory of the University of Tennessee and the Oak Ridge National Laboratory provide extensive tables of thermal properties for 200 linear polymers and small molecules. The tables can give values for temperatures from 0.1 to 1000° Kelvin. Experimental versus calculated values are clearly marked. Information is provided on both solids and polymer melts.

3) *Dielectric Constant Reference Guide (http://www.asiinstr.com/technical/Dielectric%20Constants.htm)*
Although this resource from ASI Instruments covers only one property, it is included because of the great variety of substances covered, about 1,500. Where else can one readily find the dielectric constant for beeswax or barley flour? For materials with variable compositions such as polymers or minerals, a range of values is given. This is helpful in establishing the variation that might be expected in measuring a specific sample.

4) *Pesticide Fact Sheets - New Active Ingredients (http://www.epa.gov/opprd001/factsheets/)*
This Web site contains extensive information on new pesticides registered with the U.S. EPA Office of Pesticide Programs. Since it covers only new active ingredients since fiscal year 1997, the file is small, only forty-two substances at this writing. However, as time goes on, it will grow in size and value. The fact sheets are listed by common name and can be over ten pages long. In addition to providing up to sixteen physical properties, the fact sheets provide use patterns, formulations, extensive toxicology information, and environmental fate.

5) *Phase Diagrams Web [Georgie Institute of Technology – no longer available]*

F. *Academic Directories*

The following university library Web pages access a searchable directory or contain at least some links to public Web sites in addition to their own print collection. However, even the indexes to their local print collection can be very useful, since a searcher may well have access to some of these same

resources at their location. Consider this listing to be representative, as many large universities maintain extensive Web directories in the sciences.

TABLE 6 - Evaluated Web Sites: Academic Directories

Academic Directories Web Site Name	**# of compds**	**Max. # props**	Name	CAS RN	MF	MW	Prop Values	Substruct.	**Type**	**Sponsoring Organization**
Arizona State Univ. Index to Physical, Chemical, & Other Property Data		480							Directory	Arizona State Univ.
Duke Univ. Chemical & Physical Properties in the Library		69							Directory	Duke Univ.
Indiana Univ. CHEMINFO SIRCh Physical Properties									Directory	Indiana University
Univ. at Buffalo Materials Properties Locator Database			x						Searchable Directory	Univ. at Buffalo
Univ. of Texas Thermodex		160	x						Searchable Directory	Univ. of Texas
Vanderbilt Univ. Finding Chemical & Physical Properties		120							Directory	Vanderbilt Univ.

1) *Arizona State University Index to Physical, Chemical, and Other Property Data* (*http://www.asu.edu/lib/noble/chem/property.htm*)

This Web page starts with a brief, but well chosen, list of general reference sources and then provides a list of over 400 properties with live Web links or print citations. The presentation of the information is exceptionally clear with numerous cross-references.

2) *Duke University Chemical & Physical Properties in the Library* (*http://library.duke.edu/research/subject/guides/chemical-physical-properties/*

The Duke University properties page focuses on local print sources for sixty-nine properties. However, the few Web links provided are certainly appropriate.

3*) Indiana University CHEMINFO SIRCh Physical Properties* (*http://www.indiana.edu/~cheminfo/ca_ppi.html*)

Any one spending any time in the field of chemical information quickly becomes familiar with this premier scientific information Web site maintained by Gary Wiggins of Indiana University. Though annotations are limited, the page is well organized. Many of the Web sites reviewed in this article are listed on this page. Of special value is the ability to keyword search across the entire CHEMINFO site and a back-of-the-book alphabetical index to the site.

4) *University at Buffalo Materials Properties Locator Database* (*http://libweb.lib.buffalo.edu/sel/searchSelMaterials.html*)

A searchable database of nearly 100 print sources is maintained by the Science and Engineering Library. The database record for each source contains a brief annotation, generic and specific property keywords, and types of material covered. An attempt was made to index every property covered in the source.

5) *University of Texas Thermodex http://thermodex.lib.utexas.edu/)*

This also is a searchable directory focusing on thermodynamic properties and is maintained by the Mallet Chemistry Library. The search form also allows specification of classes of materials and specific

compounds in combination with desired properties. A few publicly available Web sites are included in addition to the print sources.

6) *Vanderbilt University Finding Chemical & Physical Properties* (*http://www.library.vanderbilt.edu/science/chem/property.html*)

This is an extensive and easy-to-navigate Web directory arranged by over 100 physical properties. Free and subscription Web sources are included along with the print sources under each property. Unfortunately, there is no designation as to which Web links are subscription, i.e. available only to Vanderbilt patrons, and which are free.

CONCLUSIONS

The thirty Web sites reviewed in this article provide an impressive and useful array of physical property information. For finding common properties, the value of material safety data sheets and other company technical literature has been described. However, subscription databases can provide as much as 2.5 times as many properties for a given compound compared to a search of the free-of-charge Web sites. Physical property information on the Web is widely dispersed, requiring a patient and systematic search of numerous resources.

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