SOURCES OF PHYSICAL AND CHEMICAL DATA

In addition to the primary research journals, there are many useful sources of property data of the type contained in the *CRC Handbook of Chemistry and Physics.* A selected list of these is presented here, with emphasis on print and electronic sources whose contents have been subject to a reasonable level of quality control.

A. Data Journals

1. ***Journal of Physical and Chemical Reference Data*** – Published jointly by the National Institute of Standards and Technology and the American Institute of Physics, this quarterly journal contains compilations of evaluated data in chemistry, physics, and materials science. It is available in print and on the Internet. [ojps.aip.org/jpcrd/]
2. ***Journal of Chemical and Engineering Data*** – This bimonthly journal of the American Chemical Society publishes articles reporting original experimental measurements carried out under carefully controlled conditions. The main emphasis is on thermochemical and thermophysical properties. Review articles with evaluated data from the literature are also published. [pubs.acs.org/journals/jceaax/index.html]
3. ***Journal of Chemical Thermodynamics*** – This journal publishes original research papers that include highly accurate measurements of thermodynamic and thermophysical properties. [www.sciencedirect.com/science/journal/00219614]
4. ***Atomic Data and Nuclear Data Tables*** – This is a bimonthly journal containing compilations of data in atomic physics, nuclear physics, and related fields. [www.sciencedirect.com/science/journal/0092640x]
5. ***Journal of Phase Equilibria and Diffusion*** – This journal presents critically evaluated phase diagrams and related data on alloy systems. It is published by ASM International and is the successor to the previous ASM periodical *Bulletin Of Alloy Phase Diagrams.* [www.asm-intl.org]

B. Data Centers

This section lists selected organizations that perform a continuing function of compiling and critically evaluating data in specific fields of science.

1. **National Institute of Standards and Technology** – Under its Standard Reference Data program, NIST supports a number of data centers in chemistry, physics, and materials science. Topics covered include thermodynamics, fluid properties, chemical kinetics, mass spectroscopy, atomic spectroscopy, fundamental physical constants, ceramics, and crystallography. Address: Office of Standard Reference Data, National Institute of Standards and Technology, Gaithersburg, MD 20899 [www.nist.gov/srd/].
2. **Thermodynamics Research Center** – Now located at the National Institute of Standards and Technology, TRC maintains an extensive archive of data covering thermodynamic, thermochemical, and transport properties of organic compounds and mixtures. Data are distributed in both print and electronic form. Address: Mail code 838.00, 325 Broadway, Boulder, CO 80305-3328 [www.trc.nist.gov] .
3. **Design Institute for Physical Property Data** – Under the auspices of the American Institute of Chemical Engineers [www.aiche.org/dippr/], DIPPR offers evaluated data on industrially-important chemical compounds. The largest project deals with physical, thermodynamic, and transport properties of pure compounds. Address: Brigham Young University, Provo, UT 84602 [dippr.byu.edu] .
4. **Dortmund Data Bank** – Maintains extensive databases on thermodynamic and transport properties of pure compounds and mixtures of industrial interest. The data are distributed through DECHEMA, FIZ CHEMIE, and other outlets. An abbreviated database system is also available for educational use. Address: DDBST GmbH, Industriestr. 1, 26121 Oldenburg, Germany [www.ddbst.de].
5. **Cambridge Crystallographic Data Centre** – Maintains the Cambridge Structural Database of over 330,000 organic compounds. The data files and manipulation software are distributed in several ways. Address: 12 Union Rd., Cambridge CB2 1EZ, UK [www.ccdc.cam.ac.uk].
6. **FIZ Karlsruhe** – In addition to many bibliographic databases, FIZ Karlsruhe maintains the Inorganic Crystal Structure Database in collaboration with the National Institute of Standards and Technology. The ICSD contains the atomic coordinates and related data on over 50,000 inorganic crystals. Address: Fachinformationszentrum (FIZ) Karlsruhe, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany [www.fiz-karlsruhe.de].
7. **International Centre for Diffraction Data** – Maintains and distributes the Powder Diffraction File (PDF), a file of x-ray powder diffraction patterns used for identification of crystalline materials. The ICDD also distributes the NIST Crystal Data file, which contains lattice parameters for over 235,000 inorganic, organic, metal, and mineral crystalline materials. Address: 12 Campus Blvd., Newton Square, PA 19073-3273 [www.icdd.com].
8. **Research Collaboratory for Structural Bioinformatics** – Maintains the Protein Data Bank (PDB), a file of 3-dimensional structures of proteins and other biological macromolecules. Address: Department of Chemistry and Chemical Biology, Rutgers University, 610 Taylor Road, Piscataway, NJ 08854-8087 [www.rcsb.org].
9. **Toth Information Systems** – Maintains the Metals Crystallographic Data File (CRYSTMET). Address: 2045 Quincy Ave., Gloucester, ON, Canada K1J 6B2 [www.toth-canada.com].
10. **Atomic Mass Data Center** – Collects and evaluates high-precision data on masses of individual isotopes and maintains a comprehensive database. Address: C.S.N.S.M (IN2P3-CNRS), Batiment 108, F-91405 Orsay Campus, France [www.nndc.bnl.gov/amdc].
11. **Particle Data Group** – International center for data of high-energy physics; maintains database of properties of fundamental particles, which is published in both print and electronic form. Address: MS 50-308, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 [pdg.lbl.gov].
12. **National Nuclear Data Center** – Maintains databases on nuclear structure and reactions, including neutron cross

sections. The NNDC is the U. S. node in an international network of nuclear data centers. Address: Brookhaven National Laboratory, Upton, NY 11973-5000 [www.nndc.bnl.gov].

13. **International Union of Pure and Applied Chemistry –** Address: PO Box 13757, Research Triangle Park, NC 27709-3757 [www.iupac.org]. IUPAC supports a number of long-term data projects, including these examples:
    a. **Solubility Data Project –** Carries out evaluation of all types of solubility data. The results are published in the Solubility Data Series, whose current outlet is the *Journal of Physical and Chemical Reference Data.* [www.iupac.org/divisions/V/cp5.html].
    b. **Kinetic Data for Atmospheric Chemistry –** Maintains a comprehensive database on the kinetics of reactions important in the chemistry of the atmosphere. [www.iupac-kinetic.ch.cam.ac.uk/]
    c. **International Thermodynamic Tables for the Fluid State –** Prepares definitive tables of the thermodynamic properties of industrially important fluids. Thirteen volumes have been published by IUPAC. [www.iupac.org/publications/books/seriestitles/]
    d. **Stability Constants Database –** Collection of metal-ligand stability constants and associated software. [www.acadsoft.co.uk]

C. Major Multi-Volume Handbook Series

1. ***Chapman & Hall/CRC Chemical Dictionaries* –** These originally appeared in print form as the *Dictionary of Organic Compounds, Dictionary of Natural Products,* etc. They are now published in electronic form and are available in CDROM format [www.crcpress.com] and on the Internet [www.chemnetbase.com]. The consolidated version, called the *Combined Chemical Dictionary,* has data on more than 450,000 compounds spanning all branches of chemistry. The coverage includes physical properties, biological sources, hazard information, uses, and literature references.
2. ***Properties of Organic Compounds* –** Originally published in three editions as the *Handbook of Data on Organic Compounds,* it is now in electronic form as *Properties of Organic Compounds.* The database includes about 30,000 compounds; physical properties and spectral data (mass, infrared, Raman, ultraviolet, and NMR) are covered. It is offered as CDROM [www.crcpress.com] and web access [www.chemnetbase.com].
3. ***Beilstein Handbook of Organic Chemistry* –** The classic source of data on organic compounds, dating from the 18th century, *Beilstein* was converted to electronic form in the last decade of the 20th century. Over 8 million compounds and 5 million chemical reactions are now covered, with a broad range of physical properties as well as synthetic methods and ecological data. The database is accessed by the CrossFire software [www.mdli.com].
4. ***Gmelin Handbook of Inorganic and Organometallic Chemistry* –** A subset of the information in the print series has been converted to electronic form and is now distributed in the same manner as *Beilstein.* In addition to the standard physical properties, the coverage includes a wide range of optical, magnetic, spectroscopic, thermal, and transport properties for about 1.4 million compounds [www.mdli.com].
5. ***DECHEMA Chemical Data Series* –** DECHEMA distributes the DETHERM database, which emphasizes data used in process design in the chemical industry, including thermodynamic and transport properties of about 20,000 pure compounds and 90,000 mixtures. Access is available through in-house databases and via the Internet. [www.dechema.de].
6. ***Landolt-Börnstein Numerical Data and Functional Relationships in Science and Technology*** - *Landolt-Börnstein* covers a very broad range of data in physics, chemistry, crystallography, materials science, biophysics, astronomy, and geophysics. Hard-copy volumes in the New Series (started in 1961) are still being published, and the entire New Series is now accessible on the Internet [www.landolt-boernstein.com].

D. Selected Single-Volume Handbooks

The following handbooks offer broad coverage of high-quality data in a single volume. This list is only representative; an extensive listing of handbooks in all fields of science may be found in *Handbooks and Tables in Science and Technology, Third Edition* (Russell H. Powell, ed., Oryx Press, Westport, CT, 1994).

1. ***American Institute of Physics Handbook* –** Although an old book, it contains much data that is still useful, especially in acoustics, mechanics, optics, and solid state physics. (Dwight E. Gray, ed., McGraw-Hill, New York, 1972)
2. ***Constants of Inorganic Substances*** - This book presents physical constants, thermodynamic data, solubility, reactivity, and other information on over 3000 inorganic compounds. Since it draws heavily on Russian literature, it contains a great deal of data that does not make its way into most U. S. handbooks. (R. A. Lidin, L. L. Andreeva, and V. A. Molochko, Begell House, New York, 1995)
3. ***Handbook of Chemistry and Physics* –** Now in the 84th Edition, the *CRC Handbook* covers data from most branches of chemistry and physics. The annual revisions permit regular updating of the information. Also available on CDROM [www.crcpress.com] and the web [hbcpnetbase.com]. (David R. Lide, ed., CRC Press, Boca Raton, FL, 2002)
4. ***Handbook of Inorganic Compounds* –** This book covers physical constants and solubility for about 3300 inorganic compounds. Also available on CDROM [www.crcpress.com]. (Dale L. Perry and Sidney L. Phillips, eds., CRC Press, Boca Raton, FL, 1995)
5. ***Handbook of Physical Properties of Liquids and Gases* –** This is a valuable source of data on all types of fluids, ranging from liquid and gaseous hydrocarbons to molten metals and ionized gases. Detailed tables of physical, thermodynamic, and transport properties are given for temperatures from the cryogenic region to 6000 K. Both Western and Russian literature is covered. (N. B. Vargaftik, Y. K. Vinogradov, and V. S. Yargin, Begell House, New York, 1996)
6. ***Handbook of Physical Quantities* –** The range of coverage is somewhat similar to the *CRC Handbook of Chemistry and Physics,* but with a stronger emphasis on physics than on chemistry. Solid state physics, lasers, nuclear physics, geophysics, and astronomy receive considerable attention. (Igor S. Grigoriev and Evgenii Z. Meilikhov, eds., CRC Press, Boca Raton, FL, 1997)
7. ***Kaye & Laby Tables of Physical and Chemical Constants* –** *Kaye & Laby* dates from 1911, and the 16th Edition was

prepared in 1995 by a committee of experts. The coverage extends to almost every field of physics and chemistry; data on a limited number of representative substances or materials are given for each topic. (Longman Group Limited, Harlow, Essex, UK, 1995)

8. ***Lange's Handbook of Chemistry*** –Provides broad coverage of chemical data; last updated in 1998. Also available on the web [www.knovel.com]. (John A. Dean, ed., McGraw-Hill, New York, 1998)
9. ***Recommended Reference Materials for the Realization of Physicochemical Properties*** – This IUPAC book emphasizes highly accurate data on substances and materials that can be used as calibration standards. It covers physical, thermal, optical, and electrical properties. (K. N. Marsh, ed., Blackwell Scientific Publications, Oxford, 1987)
10. ***The Merck Index*** – Now in its 13th Edition (published in 2001), The Merck Index is a widely used source of data on over 10,000 compounds, chosen particularly for their importance in biology, medicine, and ecology. A short monograph on each compound gives information on the synthesis and uses as well as physical and toxicological properties. Also available on CDROM [www.camsoft.com]. (Maryadele J. O'Neil, ed., Merck & Co., Whitehouse Station, NJ, 2001)

E. Summary of Useful Web Sites for Physical and Chemical Properties

Most of the web sites in the following list provide direct access to factual data on physical and chemical properties. However, the list also includes portals that link to different property databases or describe the procedure for gaining access to electronic sources of property data. There are also a few chemical directory sites, which are useful for obtaining formulas, synonyms, and registry numbers for substances of interest.

Web Site	Address	Comments
Acronyms and Symbols	www3.interscience.wiley.com/stasa/	Free service; useful for identifying acronyms for chemicals
Advanced Chemistry Development	www.acdlabs.com	Chemical directory, with programs for estimating physical and spectral properties
Alloy Center	products.asminternational.org/alloycenter/	Physical, electrical, thermal, and mechanical properties of alloys
American Mineralogist Crystal Structure Database	www.geo.arizona.edu/AMS/amcsd.php	Lattice constants of minerals
Atomic Mass Data Center	www.nndc.bnl.gov/amdc/	See B.10
Beilstein	www.mdli.com	See C.3
Biocatalysis/Biodegradation Database	umbbd.ahc.umn.edu/	Biocatalytic reactions, biodegradation of chemical compounds
BioCyc	biocyc.org/	Metabolic pathways of microorganisms
BioInfo Bank	gibk26.bse.kyutech.ac.jp/jouhou/jouhoubank.html	Portal to ProTherm (protein thermodynamics), ProNit (protein-nucleic acid interactions), biomolecule structures, etc.
Biological Macromolecule Crystallization Database	www.cstl.nist.gov/biotech/carb/gilliland-group/database/database/html	Crystal data and crystallization conditions for proteins, nucleic acids, and complexes
BRENDA	www.brenda.uni-koeln.de	Enzyme nomenclature and properties
Cambridge Structural Database	www.ccdc.cam.ac.uk	See B.5
Ceramic Properties Databases	www.ceramics.org/cic/propertiesdb.asp	Mechanical, thermal, and other properties of ceramic materials
Chapman & Hall/CRC Combined Chemical Dictionary	www.chemnetbase.com/scripts/ccdweb.exe	See C.1
ChemExper	www.chemexper.com/	Consolidated chemical catalogs from various suppliers; provides physical properties and safety data; links to molfiles and MSDS
Chemfinder	www.chemfinder.com	Chemical directory, with links to several property databases
Chemical Acronyms Database	www.oscar.chem.indiana.edu/cfdocs/libchem/acronyms/ acronymsearch.html	Useful for associating chemical names and acronyms
ChemIDplus	chem.sis.nlm.nih.gov/chemidplus/	Chemical directory
ChemIndustry	www.chemindustry.com/chemicals/	Chemical directory
CHEMnetBASE	www.chemnetbase.com/content/databases	Portal to C&H/CRC Chemical Dictionaries, Handbook of Chemistry and Physics, Properties of Organic Compounds, etc.
ChemWeb Databases	www.chemweb.com/databases/	Portal to many databases
CODATA Home Page	www.codata.org	Thermodynamic key values and fundamental constants
Crystallography Open Database (COD)	www.crystallography.net	Crystal data on 12,000 compounds

Web Site	Address	Comments
DECHEMA (DETHERM)	www.dechema.de	See C.5
DIPPR Pure Compound Database	dippr.byu.edu	See B.3
Dortmund Data Bank	www.ddbst.de	See B.4
Enzyme Nomenclature Database	www.expasy.ch/enzyme/	IUBMB nomenclature for enzymes
European Bioinformatics Institute	www.ebi.ac.uk/Databases/	Nucleotide and protein sequences, protein structures, enzyme nomenclature and reactions
FDM Reference Spectra Databases	www.fdmspectra.com/	Infrared, Raman, and mass spectra
FIZ Chemie Berlin	www.fiz-chemie.de	Portal to DETHERM (C.5), Dortmund Data Bank (B.4), Infotherm
FIZ Karlsruhe - ICSD	www.fiz-karlsruhe.de	See B.6
Fundamental Physical Constants	physics.nist.gov/constants	CODATA fundamental constants
Gmelin	www.mdli.com	See C.4
Handbook of Chemistry and Physics	hbcpnetbase.com	Web version of CRC Handbook
Hazardous Substances Data Bank	toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB	Physical and toxicological properties of chemicals of health or environmental importance
HITRAN Database	cfa-www.harvard.edu/hitran/	High resolution spectroscopic data for constituents of the atmosphere; parameters for calculating atmospheric transmission
Infotherm	www.fiz-chemie.de/infotherm	Physical and thermal properties of pure compounds and mixtures
International Centre for Diffraction Data	icdd.com	See B.7
International Spectroscopic Data Bank	www.is-db.org	All types of spectra, deposited by users. Access is free.
IUBMB	www.chem.qmw.ac.uk/iubmb/	Enzyme and nucleic acid nomenclature
IUPAC Home Page	www.iupac.org	See B.13
IUPAC Kinetics Data	www.iupac-kinetic.ch.cam.ac.uk/	See B.13.b
IUPAC Nomenclature Rules	www.chem.qmul.ac.uk/iupac/	Useful site for organic and biochemical nomenclature
Klotho Biochemical Compounds Declarative Database	www.biocheminfo.org/klotho/	Structure diagrams of biochemical molecules
Kovel.com	www.knovel.com	Portal to Lange's Handbook, Perry's Chemical Engineers' Handbook, etc.
Landolt-Börnstein	www.landolt-boernstein.com	See C.6
Lipidat	www.lipidat.chemistry.ohio-state.edu/	Structures and thermodynamic properties of lipids; crystal polymorphic transitions
MatWeb	www.matweb.com	Thermal, electrical, and mechanical properties of engineering materials
Metals Crystallographic Data File	www.tothcanada.com	See B.9
NASA Chemical Kinetics Data	jpldataeval.jpl.nasa.gov	Kinetic and photochemical data for stratospheric modeling
National Center for Biotechnology Information	www.ncbi.nlm.nih.gov	Portal to GenBank and other sequence databases
National Nuclear Data Center	www.nndc.bnl.gov	See B.12
National Toxicology Program	ntp-server.niehs.nih.gov	Chemical health and safety data
NIST Atomic Spectra Database	physics.nist.gov/PhysRefData/contents-atomic.html	Energy levels, wavelengths, and transition probabilities of atoms and atomic ions
NIST Ceramics Webbook	www.ceramics.nist.gov/	See B.1
NIST Chemistry Webbook	webbook.nist.gov	Broad range of physical, thermal, and spectral properties
NIST Data Gateway	srdata.nist.gov/gateway/	Portal to all NIST data systems; see B.1
NIST Physical Reference Data	physics.nist.gov/PhysRefData/	Atomic and molecular spectra, cross sections, x-ray attenuation, and dosimetry data

Web Site	Address	Comments
NLM Gateway	gateway.nlm.nih.gov/gw/Cmd	Portal to all National Library of Medicine databases
NMR Shift DB	www.nmrshiftdb.org	NMR data submitted by users
Nucleic Acid Database	ndbserver.rutgers.edu/	Crystal structures of nucleic acids
Particle Data Group	pdg.lbl.gov	See B.11
Polymers - A Property Database	www.polymersdatabase.com/	Properties of commercial polymers
Powder Diffraction File	www.icdd.com	See B.7
Properties of Organic Compounds	www.chemnetbase.com/scripts/pocweb.exe	See C.2
Protein Data Bank	www.rcsb.org	See B.8
Sigma-Aldrich	www.sigmaaldrich.com/	Chemical catalogs; includes some physical property data
SpecInfo	www3.interscience.wiley.com/cgi-bin/mrwhome/109609148/HOME	IR, NMR, and mass spectra
Spectra Online	www.ftirsearch.com	FTIR and Raman spectra
SPRESI-web	www.spresi.de/	Structures, reactions, and some physical properties
STN Easy	stneasy.cas.org	Chemical directory (and access to Chemical Abstracts)
STN Easy-Europe	stneasy.fiz-karlsruhe.de	European node of STN Easy
STN Easy-Japan	stneasy-japan.cas.org	Japanese node of STN Easy
Swissprot	bo.expasy.org/enzyme/	Enzyme nomenclature and related information
Syracuse Research Corporation	www.syrres.com/esc/databases.htm	Properties of environmental interest
Table of Isotopes	ie.lbl.gov/education/isotopes.htm	Nuclear energy levels, moments, and other properties
Thermodynamics of Enzyme-Catalyzed Reactions	xpdb.nist.gov/enzyme_thermodynamics/	Equilibrium constants of biochemical reactions
Thermodynamics Research Center	www.trc.nist.gov	See B.2
TOXNET	toxnet.nlm.nih.gov	Portal to HSDB and other databases on hazardous chemicals
Wiley Interscience	www3.interscience.wiley.com/reference.html	Portal to Kirk-Othmer Encyclopedia of Chemical Technology, Ullmann's Encyclopedia of Industrial Chemistry, Encyclopedia of Reagents for Organic Synthesis, SpecInfo Database, etc.